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DUST

Disposal Unit Source Term

Data Input Guide

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Data Input Guide

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NUCLEAR WASTE AND MATERIALS TECHNOLOGY
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ABSTRACT

Performance assessment of a low-level waste (LLW) disposal facility begins with an estimation of the rate at which radionuclides migrate out of the facility (i.e., the source term). The focus of this work is to develop a methodology for calculating the source term. This work helps support activities to develop further guidance in the performance assessment area. In general, the source term is influenced by the radionuclide inventory, the wasteforms and containers used to dispose of the inventory, and the physical processes that lead to release from the facility (fluid flow, container degradation, wasteform leaching, and radionuclide transport). Many of these physical processes are influenced by the design of the disposal facility (e.g., infiltration of water). The complexity of the problem and the absence of appropriate data prevent development of an entirely mechanistic representation of radionuclide release from a disposal facility. Typically, a number of assumptions, based on knowledge of the disposal system, are used to simplify the problem. This has been done and the resulting models have been incorporated into the computer code DUST (Disposal Unit Source Term). This document presents the models used to calculate release from a disposal facility, verification of the model, and instructions on the use of the DUST code. In addition to DUST, a preprocessor, DUSTIN, which helps the code user create input decks for DUST and a post-processor, GRAFXT, which takes selected output files and plots them on the computer terminal have been written. Use of these codes is also described. In using DUST, as with all computer models, the validity of the predictions relies heavily on the validity of the input parameters. Often, the largest uncertainties arise from uncertainty in the input parameters. Therefore, it is crucial to document and support the use of these parameters. The DUST code, because of its flexibility and ability to compute release rates quickly, will be extremely useful for screening to determine the radionuclide released at the highest rate, parameter sensitivity analysis and, with proper choice of the input parameters, provide upper bounds to release rates.

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EXECUTIVE SUMMARY

The U.S. Nuclear Regulatory Commission (NRC) Regulation 10 CFR Part 61, "Licensing Requirements for Land Disposal of Radioactive Waste," requires that after disposal of low-level wastes (LLW) there is reasonable assurance that the general public will not receive annual off-site doses in excess of 25 millirems to the whole body, 75 millirems to the thyroid, and 25 millirems to any other organ.

Demonstration that these regulatory limits are not exceeded requires the quantitative assessment of the potential radiological impact of a LLW disposal facility on the surrounding environment. Evaluation of these impacts is accomplished through a performance assessment which includes estimates of the following processes for each radionuclide: (a) the rate of release from the disposal unit (i.e., the source term); (b) the transport from the disposal unit to the accessible environment; and (c) the conversion of the radionuclide concentration at the receptor site into an equivalent dose.

The objective of this project is to provide a computer model that estimates the radionuclide release rate from the disposal facility, that is, the source term. General guidelines used while developing the computer model included: use of a modular structure to allow further refinements, limiting the complexity of the models to permit the code to be capable of running quickly on a desktop computer system, and including the flexibility to handle a wide variety of situations typically encountered in LLW disposal.

In general, the source term is influenced by the radionuclide inventory and its origin (i.e., waste stream), the wasteforms and containers used to dispose of the inventory, and the physical processes that lead to release from the facility. The complexity of the problem and the absence of appropriate data prevent development of an entirely mechanistic representation of radionuclide release from a disposal facility. Typically, a number of assumptions, based on knowledge of the disposal system, are used to simplify the problem. The assumptions used while selecting the models to represent radionuclide release from the disposal facility and the rationale for these assumptions was presented in a previous report in this program [Sullivan, 1991a].

The models selected to represent the four major processes (fluid flow, container degradation, wasteform leaching, and radionuclide transport) influencing release have been incorporated into the computer code DUST, Disposal Unit Source Term, and are described in this report.

The DUST code permits the user to select from two different methods of calculating the transport of radionuclides through the facility, the Multi-Cell Mixing Cascade (MCMC) model and the one-dimensional finite difference (FD) model. The MCMC model is an analytical solution of the advective transport equation with radioactive decay and chemical retardation for constant flow and material properties. The model does permit a unique time to container failure and wasteform release rate for each mixing cell having a container. The MCMC model requires relatively little computer time to operate. The FD model solves the transport equation with the processes of advection, dispersion, retardation, and radioactive decay. It is capable of modeling a wider range of conditions than the MCMC model as it permits non-uniform flow and material properties, however, it requires

substantially more input and computer time. A complete discussion of the differences between the two models is presented in this report.

The DUST code models fluid flow through tabular input of the flow velocity versus time when using the FD model. For the MCMC model, a time-independent flow velocity must be specified.

Container degradation is modeled in both transport models through a unique container failure time. The value for this parameter should be selected based on the materials and expected environment. In addition, the FD model permits localized container failure. In the localized failure model, a fraction of the container becomes breached prior to total failure. This permits an earlier release of contaminants from the wasteform.

Wasteform release is modeled through three release mechanisms: a surface rinse process in which radionuclides are released upon contact with the solution, partitioning between the wasteform and solution can be modeled when using the FD transport model; diffusion controlled release from the wasteform (FD transport model only); and uniform release in which a fixed fraction of the inventory is released every year. All of these release mechanisms account for radioactive decay of the source. In addition, for the uniform and surface rinse mechanisms a check is performed to insure that releases do not cause concentrations to exceed a user defined solubility limit.

To ease the burden of creating an input deck a pre-processor, DUSTIN, was written. DUSTIN is a menu driven program that guides the user through all of the necessary steps of creating an input deck. Use of DUSTIN permits the user to create an input deck without knowing the formatted structure used by the DUST code. A complete description of DUSTIN and its operation is provided in this report. To allow direct modification of an input deck, a complete description of the formatted structure of a DUST input deck is also provided.

To facilitate the analysis of the output from the code, the program GRAFXT was written. GRAFXT is a menu driven program that reads files created by DUST and plots the data on a video display unit. Graphs of the concentration, flux, and total mass that has passed through a region can be displayed as a function of time or spatial location.

The DUST code has received extensive testing and verification. DUST code predictions have been compared to known analytical solutions as well as other code predictions. A discussion of several of these verification tests is provided.

The DUST code improves upon existing models in that more flexibility is allowed in modeling the various waste stream/wasteform/container systems while still retaining relatively simple models that do not require extensive computer time or provide an undue burden on the code user in terms of input requirements. However, the models used within the DUST code are based on a number of assumptions. A complete discussion of the limitations that result from the assumptions is presented.

In using DUST, as with all computer models, the validity of the predictions relies heavily on the validity of the input parameters. Often, the largest uncertainties arise from uncertainty in the input parameters. Therefore, it is crucial to document and support the use of these parameters.

The DUST code, because of its ability to compute release rates quickly, will be extremely useful for screening to determine the radionuclides released at the highest rate, parameter sensitivity analyses, and, with proper choice of the input parameters, provide upper bounds to release rates.

1. INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC) issued the regulation 10 CFR Part 61, "Licensing Requirements for Land Disposal of Radioactive Waste" [FR, 1982]. 10 CFR Part 61 requires, in part, that any "proposed disposal site, disposal facility design, land disposal facility operations (including equipment, facilities and procedures), disposal site closure, and postclosure institutional control are adequate to protect the public health and safety..." Protection of the public is judged by requiring that releases which may occur must be demonstrated with reasonable assurance not to exceed an equivalent dose of "25 millirem to the whole body, 75 millirems to the thyroid, and 25 to any other organ of any member of the public." This requires the quantitative assessment of the potential impacts of a low-level radioactive waste (LLW) disposal facility on the surrounding environment. In particular, estimation of the dose to the maximally exposed individual is required.

Estimation of the dose to man is accomplished through a performance assessment. A proposed strategy for conducting such an assessment has been presented by the NRC [Starmer, 1988]. Further guidance will be provided by the NRC in their Branch Technical Position on Performance Assessment, preparation of which is in progress. Work under this project supports activities in the development of additional guidance. In the proposed performance assessment strategy, performance assessments are conducted through combining a series of separate calculations. These calculations include estimating the rate of radionuclide release from a disposal unit, (i.e., the source term), the transport of the radionuclide from the disposal unit to the accessible environment, and, finally, the conversion of the radionuclide concentration at the receptor site into an equivalent dose. Examples of this approach can be found in the reports produced for the NRC by the staff at Sandia National Laboratory [Kozak, 1989; Kozak, 1990: Chu, 1991].

The objective of this project is to provide computer models that estimate the radionuclide release rate from the disposal facility. A disposal facility is a complex, heterogeneous collection of wastes/wasteforms/containers, soils, and engineered structures (concrete vaults, backfill, vault covers, drains, etc.). For most radionuclides, release from this disposal unit is controlled by access of water to the wasteform, release from the wasteform, and transport to the disposal unit boundary. These processes are influenced by the design of the disposal unit, hydrology, geochemistry and wasteform/container characteristics. A disposal unit is schematically depicted in Fig. 1.1 and typically contains a multi-layered cover to divert water away from the waste; an engineered barrier to further reduce water flow to the wastes (for trench disposal there is no engineered barrier); and metallic, concrete, or HDPE waste containers. The waste comes in many forms including solidified in cement, dewatered resins, activated metals, dry solids (e.g. contaminated paper, cloth, rubber, plastic, glass, etc.).

Figure 1.1 Schematic diagram of a LLW Disposal Unit.

The heterogeneity and complexity of the disposal facility make development of a three-dimensional time-dependent model that covers all possible physical and chemical conditions an extremely cumbersome and difficult task. Even if one could develop models for all conditions, their applicability would be restricted by data limitations and the extensive computer time that would be needed.

Therefore, simplifications are justified. The simplified models should account for the most important physical processes and parameters influencing release while retaining as much accuracy as possible. Further, the models should be flexible enough to simulate the wide range of anticipated conditions and not be overly conservative.

Previous reports on this program, [Sullivan, 1991b; Cowgill, 1992; Cowgill, 1992a], presented a review of waste disposal practices, physical and chemical processes that influence release from the facility, reviewed other source term modeling efforts, and recommended models for incorporation into a source term computer model. These models have been embodied into the computer code DUST, Disposal Unit Source Term.

Chapter 2 provides a description of the mathematical models and governing equations used to represent water flow, container degradation, wasteform leaching, and contaminant transport. A discussion of the range of the parameters in the various models is also provided.

Chapter 3 discusses the procedure used to operate the DUST code. In addition to DUST, a pre-processor, DUSTIN, was written to assist the code user in creating an input deck and a post-processor, GRAFXT, was written to take output files generated by DUST and plot them on the video display unit.

Chapter 4 discusses the limitations of the models.

Several test problems with known analytical solutions have been simulated with the DUST code. The results of these verification tests are presented in Chapter 5.

Chapter 6 presents detailed instructions on how to use the pre-processor DUSTIN. This code is menu driven and asks the user for all of the variables needed to run DUST. DUSTIN will take this information and write it to a file in the form required by DUST, thereby, eliminating the need to know the exact structure of an input file. This chapter also discusses the input parameters and provides guidance on their selection.

Chapter 7 discusses the format of the input required by DUST. This permits the user to create or modify an input deck without using DUSTIN. Sample input decks are provided and discussed.

Chapter 8 discusses the various output files created by DUST. In addition to the main output file, which contains the problem definition and the requested output (concentrations, fluxes, and wasteform mass release rates), DUST creates files containing concentration, flux, or total mass that has moved past a given location for use with GRAFXT, and files containing information on the wasteform release rates.

Chapter 9 discusses the use of GRAFXT, the graphics program for DUST output files, TRACECND.DAT, TRACEFXD.DAT, and CONCNT.DAT.

Chapter 10 provides a brief summary and conclusion for this report.

2. MODEL SELECTION AND GOVERNING EQUATIONS

A LLW disposal unit is a complex, heterogeneous collection of wastes/ wasteforms/containers, soils, and engineered structures (clay caps, concrete vaults, drains, etc.). Aqueous release of radionuclides from this disposal unit is controlled by water flow, access of the water to the wasteform, release of the radionuclide from the wasteform, and transport to the disposal unit boundary. These processes are influenced by the design of the disposal unit, precipitation, hydrology, geochemistry, and wasteform/container characteristics. To model the complete disposal unit, including every waste container individually would require a three dimensional model that considered all of these processes simultaneously. Such a model does not exist today. Even if such a model did exist, its use would require extensive computing times and the accuracy of the predictions would be questionable due to limitations in the data.

Therefore, simplifications from a fully descriptive three-dimensional model are justified. These "simplified" models are a necessary step in developing predictions of the behavior of a LLW disposal site.

The "simplified" models incorporated into DUST account for the most important physical processes and parameters influencing release. Further, the models are flexible enough to simulate a wide range of conditions. For example, multiple container failure and wasteform release rates can be modeled.

The DUST code has been developed in a general manner which allows simulation of the majority of situations expected to occur. However, to account for the possibility of special cases and allow easy modifications of the models within the code to reflect new and better information, the code structure is modular.

In the following sections, the framework for the DUST code is presented. Within that framework, the models for the four processes (water flow, container degradation, wasteform release, and transport) that influence release are discussed separately. This chapter contains the basic equations that govern the release and transport within the facility . However, the detailed equations describing the analytical solutions used in modeling these processes are presented in Appendix A.

2.1 DUST Code Framework

The ultimate objective of the DUST code is to predict the rate of release of radionuclides from a shallow land disposal facility. As discussed earlier, this will be accomplished through use of computer models. These models should be simple enough to allow simulation of a large number of cases and flexible enough to allow simulation of a wide range of situations. To achieve this one can use analytical or numerical solution procedures. Analytical solutions often have the advantage of being easier to compute than numerical solutions. Numerical solutions offer the flexibility to model a wider range of conditions. For these reasons both are incorporated into the DUST code.

The DUST code was written in an attempt to achieve a balance between the use of extremely simple but conservative assumptions which lead to high predicted release rates and complicated models that include all of the known physical and chemical processes that influence release but require

extensive computer time and expertise to define the problem (select the input variables). To strike this balance, assumptions regarding which are the most important physical parameters and the level of detail needed to calculate these parameters have been made. These are discussed in detail in the model selection report [Sullivan, 1991]. Also, a pre-processor, DUSTIN, has been written to ease the burden of creating an input deck. DUSTIN is discussed in detail in Chapter 6.

The primary equation for predicting release from the disposal facility is the contaminant transport equation. In addition, there are models that supply information on fluid flow, container degradation and wasteform release. For calculating transport, two models are permitted, the Multi-Cell Mixing Cascade (MCMC) model and the Finite Difference (FD) model. A flow chart of the various subroutines that comprise the DUST code is presented in Appendix B.

The MCMC model divides the modeled domain into mixing cells. Each mixing cell has the same size and transport properties. However, container performance and wasteform release may vary between mixing cells. Using this approach, an analytical solution of concentration versus time may be obtained for any mixing cell [Sullivan, 1991]. This solution is presented in Appendix A.

The FD model divides the modeled domain into finite regions called control volumes. The FD model is a generalization of the MCMC model and permits more flexibility in modeling different situations. In particular, the FD model permits different transport properties in each node, diffusive/dispersive transport, and more general wasteform release models.

The differences between the two transport models leads to substantial differences in selection of the container degradation and wasteform release models. Therefore, the transport models are discussed first.

2.2 Radionuclide Transport

Two alternative methods have been selected to model transport within the disposal facility. The multi-cell mixing cascade (MCMC) models [Fig. 2.1] used in the PAGAN performance assessment code [Kozak, 1990; Chu, 1991] have been generalized to allow more realistic estimation of the releases from the disposal facility while still retaining an analytical solution procedure. In cases where the assumptions used in obtaining the analytical solutions are not appropriate, a one-dimensional finite difference (FD) model is provided.

Figure 2.1 Schematic representation of the mixing cell cascade approach. (a) a single mixing cell, (b) multiple mixing cells. [From Kozak, 1990]

Both models begin with the one-dimensional advection-dispersion transport equation:

$$\frac{\partial}{\partial t}(\theta C) = \frac{\partial}{\partial x}\theta D\frac{\partial C}{\partial x} - \frac{\partial}{\partial x}V_D C$$

$$+ q$$
$$- \lambda(\theta C + \rho S) - \frac{\partial}{\partial t}(\rho S)$$

where:

C = solution concentration;
θ = the volumetric moisture content of the region (dimensionless);

$$D = D_{eff} + \frac{a_l |V_D|}{\theta};$$

D = the diffusion-dispersion coefficient,
D_{ef} = effective diffusion coefficient;
a_l = dispersivity coefficient;
V_D = Darcy velocity;
λ = radioactive decay constant;
S = adsorbed concentration, the mass adsorbed per unit mass of the solid;
ρ = bulk density of the solid; and
q = source/sink term used to model release from the wasteform and external sources, e.g., production due to radioactive decay.

In Eqn. (2.1) we assume that the mass adsorbed on the solid surfaces is in equilibrium with the mass in solution. Further, we assume that this equilibrium can be described using a concentration independent distribution coefficient, K_d, as follows:

$$S = K_d C$$

Using the above relationship for S, assuming that the bulk density remains constant within the disposal facility and rearranging Eqn. (2.1), the following equation is obtained:

$$\frac{\partial}{\partial t}(R\theta C) = \frac{\partial}{\partial x}\left(\theta D\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(V_D C) - \lambda\theta R C + q$$

where:

$$R = 1 + \frac{\rho K_d}{\theta}$$

R is known as the retardation coefficient. Values of the distribution coefficient (K_d) are known to change by orders of magnitude under different chemical conditions. Therefore, the value selected for K_d must be well supported. Typical K_d values for a range of conditions have been compiled in several reports [Thibault, 1990; Looney, 1987; Baes, 1983].

2.2.1 FD Model

The FD model takes Eqn. (2.3) and transforms it into a set of coupled algebraic equations using a control volume approach. In this method, the modeled domain is divided into control volumes. A mass balance is performed for each control volume through approximation of the derivative terms in Eqn. (2.3) using finite differences. The time derivative is estimated using a backward difference procedure. The diffusion/dispersion term is estimated using central differences. The advection term is modeled using an upwind difference. A complete description of the control volume approach and the resulting system of equations is presented in Appendix A.

The FD model is quite general in that in principle each control volume could have a different retardation coefficient, diffusion/dispersion term, moisture content, and source/sink term. (In practice, DUST permits only 10 different material types per calculation.) This flexibility permits simulating the effects of caps, engineered barriers, and backfill using different parameters. In addition, the source/sink term contains two components, a wasteform term and an external term. The wasteform term is calculated using the release models described in Section 2.5.

In the MCMC model, migration is permitted only through advection altered through the effects of retardation in the downward direction. As stated previously, the mixing cell cascade model does not model diffusional or dispersive transport and does not allow for migration up towards the surface. Diffusional transport may be an important process during the time period when the engineered barriers provide protection against water flowing through the waste containing region of the trench. Dispersion may be important in causing early releases and in spreading the contaminant causing lower peak concentrations.

2.2.2 Mixing-Cell Cascade

The mixing cell cascade model divides the disposal facility into a number of uniform size mixing cells as depicted in Figure 2.1. Within each cell it is assumed that the contaminant released from the waste form is uniformly mixed thereby giving a uniform solution concentration. In order to obtain an analytical solution the following assumptions are made:

a) Migration is dominated by advective flow and therefore diffusion and dispersion can be ignored.

b) The advection velocity, moisture content, and the retardation coefficient are constant throughout the disposal facility. Although these parameters will show variations due to different materials in the facility, they should be selected to provide a representative average for the entire facility. Obtaining a time-independent average value for the retardation coefficient in a multi-layered system is not a trivial task. Examining Eqn. (2.5) it is seen that during a transient, the importance of the retardation coefficient depends on the gradient in concentration which changes in time. As an example, consider a problem that has a source at the boundary and two different material regions. At times prior to the contaminant arriving in region 2, the effective system retardation coefficient is that of material 1. As contaminant enters region 2, its transport characteristics play a role in determining migration and the effective retardation coefficient becomes a function of the region 1 and 2 values. At later times, if region 1 obtains a quasi-steady state ($\partial c/\partial t \approx 0$), the retardation coefficient in this region becomes unimportant and the system retardation coefficient would be close to that in region 2. In general, if the retardation coefficient within the disposal facility varies greatly from region to region, it is recommended to use the FD transport model.

Using these assumptions in Eqn. (2.3) the transport equation for the i^{th} mixing cell becomes:

$$\frac{\partial C_i}{\partial t} = -\frac{V_D}{\theta R}\frac{\partial C_i}{\partial x} - \lambda C_i + \frac{q_i}{\theta R}$$

where the subscript i refers to the i^{th} mixing cell.

For a disposal facility of height H, there are N mixing cells of height h (h = H/N). Using this definition of the size of the mixing cell and upwind differencing (because migration is assumed to be controlled by advection) to estimate the spatial derivative, Eqn. (2.5) becomes:

$$\frac{d C_i}{d t} = -\alpha N (C_i - C_{i-1}) - \lambda C_i + \beta N Q_i$$

where:

Q = the total release rate from the wasteform;
α = $V_d/(\theta R H)$;
β = $1/(\theta R H A_f)$; and
A_f = the area of the facility.

In this description, HA_f/N is the volume of a single mixing cell.

Equation (2.6) applies to each mixing cell. For the first cell, C_{i-1} is set to zero. This is equivalent to assuming that no contaminant enters through the top of the facility. Therefore, we have a system of N coupled linear differential equations. This system of equations has been solved to provide an analytical solution for arbitrary wasteform sources, Q_i, within each mixing cell. The results are presented in Appendix A.

A control volume in the FD approach is equivalent to a mixing cell in the MCMC approach. Often throughout the remainder of this document, the term node is used. This is a generic term for the region of computational interest, i.e., a node can refer to either a mixing cell or control volume. Where possible, the term control volume will be used for cases that apply only to the FD model, mixing cell will be used only for cases involving the MCMC model, and node will be used in cases that apply to both models.

2.3 Fluid Flow

Although setting a disposal facility beneath the water table is permitted, it is expected that new facilities will be located above the water table in the unsaturated zone. In either case, the most likely pathway for release will be through the water. Infiltration of water into a facility will involve many processes including precipitation, evapotranspiration, and surface run-off. Water flow in the unsaturated zone is difficult to predict due to the non-linearity of the unsaturated soil flow properties. This is further complicated by the barriers (trench cap, concrete structure, etc) any disposal facility will have to minimize infiltration into the waste containing region.

A simple model for infiltration is needed. In addition, predicting infiltration into soils in arid sites under all conditions is difficult [Gee, 1988]. To calculate flow into a disposal facility would require at least a two-dimensional simulation. Further, the flow rate will vary with time on a short time scale (hours) due to precipitation events and evapotranspiration and on a long time scale (years) due to changes caused by degradation of the infiltration barrier. To follow the evolution of water flow with time would require an extensive computing expense. Thus, this is not appropriate for the source term model.

In the DUST code, for the FD transport model, water infiltration is calculated as a function of time through tabular input.

$$V_d = F(t)$$

where V_d is the volumetric flow velocity (Darcy velocity) of the water and F(t) is defined in an input table. If the MCMC transport model is used, the Darcy velocity must be a constant.

This flow rate should be the yearly average based on the expected conditions. For advection driven transport it has been shown that the average rate of contaminant transport depends on the average flow rate [Sullivan, 1988a].

The choice of the value for the flow rate should be conservatively chosen or supported by more detailed computer simulations such as VAM2D [Huyakorn, 1989], FEMWATER [Yeh, 1987], TRACR3D [Travis, 1991], etc. If a computer simulation is not performed, an upper bound for the flow rate is the annual precipitation rate. If the evapotranspiration rate is accurately known this could be subtracted from the precipitation rate at humid sites. At arid sites this may lead to large errors in predicted recharge [Gee, 1988]. Alternatively, if the recharge rate through the disposal facility is known due to measurement at the site, this value could be used.

In the actual situation, infiltration may be very low until significant degradation of the cap occurs. If one accounts for degradation of the cap, this will require additional modeling. At this time, there is no widely accepted model for the degradation of earthen materials or engineered (i.e., concrete) caps. This is due in part to the need to predict performance over hundreds of years based on experience and data that have been collected over a period of years.

However, work is being performed to determine the degradation mechanisms of underground concrete structures. Models based on these studies are under development [Clifton, 1989; Walton, 1990; Shuman, 1991] and should help in estimating the rate of degradation. This information could then be used to calculate water flow through the degraded barrier and into the waste containing region of the disposal facility.

2.3.1 Gas Flow

If it is determined that the gaseous pathway may be significant, the flow of gas through the facility will need to be modeled. Conceptually, the DUST code would handle the problem in an identical fashion to that for water flow, i.e., a table of volumetric gas flow rate versus time could be used for the FD model and a constant value for volumetric gas flow rate could be used by the MCMC model. Models for the production and/or release of gaseous phase radionuclides would have to be developed.

The transport of gaseous radionuclides within the disposal facility requires special attention. For gases, flow may be up and out of the disposal facility or out of the bottom through drains. Upward migration will involve advection due to pressure variations that will vary seasonally and diurnally, as well as diffusion. As revealed in the review of existing source term models [Sullivan, 1991a], very little work has been performed in modeling gaseous release for performance assessment calculations.

As with water flow, prediction of the upward migration of gas is a complicated problem. Due to the length of time to be considered in a performance assessment, it is impractical to model daily or

seasonal variations in gas flow rate. Therefore, it will be necessary for the code user to supply an average gas advection velocity in order to calculate gaseous release. This flow rate should be estimated using state-of-the-art computer codes or, as a minimum, chosen to permit conservative predictions of gas release.

2.4 Container Degradation

Waste containers in the early days of LLW disposal ranged from cardboard and wooden boxes to carbon steel drums and boxes. Since the passage of 10 CFR Part 61, cardboard and wooden boxes are no longer used. As of 1988, carbon steel drums and boxes were widely used to dispose of Class A wastes, the largest volume of wastes. Most Class B and C wastes are disposed of in high-integrity containers (HIC) but a small fraction have been stabilized in cement and placed in 55 gallon drums [Sullivan, 1989]. Recently, there has been a trend to rely more and more exclusively on HIC's for Class B and C wastes due to their ease of use, lack of need for processing equipment, reduced worker exposure, problems encountered with solidification of some waste streams, and their approval by NRC as a means of demonstrating structural stability.

A waste generator has a number of different HIC's from which to choose. These include HIC's made from Ferralium 255, from stainless steels, from polymer-impregnated concrete, and high-density polyethylene (HDPE). A HIC may also have an internal lining to isolate the waste from the external barrier to water flow. The liner materials are typically polyethylene. HIC's should be designed to maintain their structural stability and maintain a positive seal for 300 years as indicated in the NRC Technical Position on Wasteform [Higginbotham, 1983; Lohaus, 1991]. Structural stability does not imply that the HIC's will remain water tight. In time, water may enter through the passive gas vents required on HIC's or through small cracks and localized failures that may occur.

Currently, most waste containers are metallic. The use of HDPE alone is suspect due to the potential of long term creep affecting its stability and it is no longer on the NRC-approved list of HIC's. HDPE is used as a liner in metallic containers and within a concrete caisson which is backfilled with soil. The Richland site received five of these concrete caisson/HDPE HIC's in 1988 [Sullivan, 1989].

Modeling of metallic corrosion on a mechanistic scale is strongly dependent on the local chemistry and quite complicated. For the source term model, the work required to perform such a calculation is not justified. Rather, in the DUST code metallic container degradation models will be semi-empirical and rely on the existing corrosion in soil data base. If internal corrosion is expected to be important, this can also be included in the empirical model, however, data in this area is lacking. In the DUST code, two types of failure are modeled: general failure, and localized failure.

2.4.1 General Failure

In the DUST code general failure is modeled through a user-specified time of failure. In this model, the container prevents water ingress to the waste until failure, at which time the container no longer provides a barrier to water flow. For metallic containers, the time to failure could be estimated as the thickness of the container divided by the time-averaged corrosion rate.

Corrosion rates should be obtained from site specific data whenever possible. When this is not possible, the data base generated by the National Bureau of Standards, NBS (currently, National Institute for Standards and Technology) [Romanoff, 1957; Gerhold, 1981] for carbon steels and stainless steels could be used for these materials. There is no data base for the corrosion of Ferralium in soil systems. However, Ferralium, a duplex stainless steel, has shown superior corrosion performance as compared to 304 and 316 stainless steels in a wide range of environments. If this trend holds for soil systems, use of the NBS data for stainless steels should be conservative.

The NBS studies of carbon steels covered a period of 17 years and 47 different soils [Romanoff, 1957]. Uniform corrosion rates in this study of carbon steels ranged from 8×10^{-4} - 2×10^{-2} cm/yr, with the mean value being 5.7×10^{-3} cm/yr. In the LLW Updated Impacts Analysis [Otzunali, 1986] the recommended value for carbon steel corrosion was 4 mils/yr (1×10^{-2} cm/yr). For typical 55 gallon carbon steel drum thicknesses, 50 mil, container lifetimes would be expected to range from 6 to 160 years with a mean lifetime of 23 years based on the above data.

The NBS studies of 304 and 316 stainless steels were conducted over 14 years in 15 soils. General corrosion rates for 304 stainless steel ranged from 1.7×10^{-5} - 1.1×10^{-7} cm/yr, with the mean value being 5×10^{-6} cm/yr [Gerhold, 1981]. Corrosion rates for 316 stainless steel ranged from 5.7×10^{-6} - 2.8×10^{-8} cm/yr, with the mean value being 1.3×10^{-7} cm/yr [Gerhold, 1981]. Otzunali recommended a value of 0.3 mils/yr (7.6×10^{-4} cm/yr) [Otzunali, 1986]. For a 3/8 inch thick stainless steel container, the lifetime based on the corrosion rate recommended by Otzunali would be 1250 years.

In the soil corrosion experiments, it was noted that corrosion rates typically decreased over time [Romanoff, 1957, Gerhold, 1981]. Provided that there is no change in the degradation mechanism, the experimentally measured decreasing corrosion rate indicates a constant rate based on short term data is likely to overpredict the total amount of corrosion.

For containers with non-metallic components (HDPE containers, polyethylene lining in metal, concrete caissons, etc.) there are few data on their long term performance. It is recommended that the general failure rate be selected in a conservative manner based on expert judgement.

Both transport models permit a unique time to failure for every container.

2.4.2 Localized Failure

The FD transport model also permits containers to partially fail prior to general failure. The analytical solution for the MCMC model does not accommodate partial container failures.

If localized failure occurs, water will contact the wasteform causing the release of radioactivity before the general corrosion allowance is reached. This solute may be released immediately after local failure or it may be stored within the container causing a large pulse type release when general failure occurs. In either event it may have a significant impact on predicted releases from the disposal facility.

For metallic HIC's localized failure can occur due to pitting, stress corrosion cracking, failure of the passive gas vents, or other mechanisms. In these failure scenarios, only a small portion of the container will permit water access to the wasteform. The reduced water flow impacts on the amount released and available for transport. This is accounted for in the leaching model.

Localized failure is modeled similarly to the approach used the BLT code [Sullivan, 1989]. The model was originally developed for pitting of carbon steel drums. The breached area is estimated from the following equation:

$$A_b = N_p A_c \pi (h^2 - T^2)$$

where:

N_p is the number of localized failures per unit area of the container;
A_c is the total container area;
T is the thickness of the metal; and
h is the penetration depth.

If the penetration depth, h, is less than the metal thickness, the container has not been penetrated and the breached area is set to zero.

$$h = kt^n$$

The penetration depth is estimated from the expression:

where t is time in years, and k and n have been determined for carbon steel [Mughabghab, 1988] based on the NBS corrosion data in soils [Romanoff, 1957; Gerhold, 1981]. For carbon steel, the parameter k was found to depend on the soil-water pH and the parameter n depends on the degree of soil aeration, moisture content, and clay content. The value for n is always less than 1 and is higher for poorly aerated soils (poor drainage) as compared to well aerated soils.

A detailed discussion of the choice of values for N_p, k and n can be found in the BLT data input guides [Sullivan, 1989], which is reproduced in Appendix C. For carbon steels, N_p was found to range from 0.05 to 0.5 per cm^2, the average value for k was 0.0457 cm/yr^n and n ranged from 0.01 to 0.93. Typical values for these parameters are discussed in Section 6.8.6.

For stainless steels, even though there are 14 years of corrosion data in 15 different soils [Romanoff, 1957; Gerhold, 1981], the data are insufficient to support estimation of the necessary parameters. Thus, for these and other container materials, the parameters will have to be estimated using engineering judgement if localized corrosion is modeled.

Through proper choice of the localized corrosion parameters, failure of the passive gas vents required on HIC's may also be modeled. For example, by setting n to zero and appropriate choice of the parameters h and N_p, a constant area of failure may be estimated. This failure area may be particularly important if gaseous release is being modeled.

Consideration should also be given to internal corrosion. HIC's may store wastes without the waste undergoing a solidification process. In this case, the wastes may directly contact the lining or, in the absence of a lining, the container material. Many LLW wastes contain corrosive agents that could possibly lead to penetration via pitting (localized failure). For example, it has been shown that resin beads in contact with stainless steel led to discoloration and pitting in short term tests [Soo, 1990].

2.5 Wasteform Leaching

Radionuclide release from the wasteform commences upon container failure. In a LLW facility there will be several different wasteforms, a partial list of which includes: wastes solidified by one of several processes (cement, VES, bitumen); activated metals; compacted lab trash; dewatered resins; liquids contained in an absorbent; and adsorbed gases [Roles, 1990]. The disposal data must be analyzed in order to determine the most likely release mechanisms for each radionuclide. After analyzing the data, each of the major categories of wasteforms should be grouped in terms of release mechanism. Review of the disposal data shows the following major waste streams:

a) activated metals;
b) dry active wastes;
c) resins; and
d) filter media

Approximately 70% of the activity is in activated metals, 15% of the activity is solidified in cement, and most of the rest is dry active wastes [Sullivan, 1991b]. However, the distribution by radionuclide changes markedly from one radionuclide to the next. For example, over 80% of the Th-

232 is disposed of with sorbents, over 50% of the C-14 is in cement, etc [Cowgill, 1992]. Therefore, the user must determine the distribution on a radionuclide specific basis.

Based on the above groups the following release mechanisms will be modeled:

a) Solubility limited;
b) Surface wash-off subject to partitioning;
c) Diffusion; and
d) Uniform (e.g., Dissolution).

In general, a wasteform may release radionuclides by more than one mechanism. This will be allowed through user-supplied input. In particular, the user will be allowed to specify the fractional amount of mass released by each mechanism. For example, the user could specify that for 10% of the mass, release is controlled by partitioning, while the other 90% is controlled by diffusion. This flexibility may prove to be important when homogenizing the number of waste streams/wasteforms or in modeling large boxes containing many wasteforms.

2.5.1 Solubility-limited Release

Solubility-limited release will be modeled by allowing an instantaneous release of radionuclides into solution until the limit is reached or the entire inventory is released. Further, if a solubility limit is specified and other release mechanisms are used to predict release, the amount released will be constrained such that the solubility limit is not exceeded. In general, the chemistry that occurs within a disposal facility is complex and changes in time due to the degradation of the waste containers and wasteforms. Obtaining reliable solubility limits in this environment is a difficult task. Any choice of solubility limits must be justified as conservative under all of the potential conditions. For this reason, the default solubility limit in the DUST code is arbitrarily set to 10 gm/cm^3. This value is high enough to insure that solubility limits do not influence release. Representative ranges of solubility limits have been compiled and are presented in [Looney, 1987].

2.5.2 Surface Rinse with Partitioning

The surface rinse model assumes that the radionuclides in the wasteforms with this release characteristic are available for release as soon as water contact occurs. Prior to container failure the radionuclides may be held on the wastes by adsorption, chemisorption, adhesion, and ion-exchange among other factors. To account for these factors a partition factor, which is an equilibrium ratio relating the amount on the wasteform to that in solution, can be used. This partition factor depends on the properties of the wasteform and the local chemistry. The partition factor is a lumped parameter that covers many physical processes. Therefore, obtaining reliable estimates may be difficult.

2.5.2.1 MCMC Model

Use of the MCMC transport model requires a single retardation coefficient representative of the entire disposal facility. Therefore, the partition coefficient in the rinse model is identical to the system distribution coefficient. It is a global parameter that reflects a system average value, accounting

for the different materials within the disposal facility (soil, wasteforms, containers, engineered barriers, etc.).

Equilibrium between the solution and the solids is assumed to occur instantly after container breach at time τ_b. One method for expressing this release rate, Q, in Eqn. (2.6) is:

$$Q = M(t)\,\delta(t - \tau_b)$$

where:

M(t) = $M_r e^{-\lambda t}/R$;
M_r = rinse mass available at t = 0;
λ = radioactive decay constant;
R = retardation coefficient = $1 + \rho K_d/\theta$;
K_d = distribution coefficient;
θ = moisture content; and
ρ = bulk density of the solids.

The model assumes that all of the rinse mass is released upon breach. Equation (2.10) calculates the amount that enters solution (the rest of the mass is adsorbed on the solids). As mass in solution is removed due to transport or decay, mass adsorbed to the solids is released to solution to maintain the local equilibrium. In the present form, Eqn. (2.10) is useful in the mixing cell cascade model which analytically integrates the release term. However, due to the δ function, it is not useful for the finite difference model.

2.5.2.2 FD Model

For the finite difference model, the mass released to solution is calculated by requiring equilibrium between the solid and solution to be maintained at the beginning of each time step. As mass is transported away over the numerical integration time step, equilibrium is no longer maintained. Therefore, the procedure is repeated at the beginning of each time step. This following expression for the mass release rate to solution arises:

$$q(t) = \frac{M(t)\left(1 - \dfrac{C}{C_{sat}}\right)}{\theta V \Delta t}$$

where:

q(t) = release rate per unit volume;

$\Delta M(t)$ = mass released at time t to maintain equilibrium;
$C(t)$ = solution concentration at time t;
V = volume of the finite difference node; and
Δt = time step size.

After performing the mass balance at the beginning of the time step, M(t) can be estimated from [Sullivan, 1991]:

$$\Delta M(t) = \frac{\left(M_r(t) - \frac{\rho K_p}{\theta} M_s(t) \right)}{\left(1 + \frac{\rho \circ K_p}{\theta} \right)}$$

where:

K_p = the wasteform partitioning coefficient. In the FD Model the soil distribution coefficient may differ from the wasteform partition coefficient. Also, each wasteform may have a unique partition coefficient.

$M_r(t)$ = the rinse mass available at time t, which is the original rinse mass minus any mass that has been released or lost to radioactive decay.

Also,

$M_s(t)$ = $C(t)\ \theta\ V$ = mass in solution at time t.

2.5.3 Diffusion Release Model (FD Model Only)

Experimental leaching data from solidified wastes often indicate that diffusion is the rate controlling process. In fact, the ANS 16.1 standard leach test interprets the data in terms of diffusion [ANS, 1986].

Diffusion-controlled release is characterized by relatively high leach rates at early times which continually decrease over time. In fact, analytically, the release rate, although it is integrable, approaches infinity as time approaches zero. For this reason, a release model based on a constant release rate may prove to be difficult to justify for diffusion controlled release. Choosing a constant release rate based on short term releases may be overly conservative while choosing the rate based on some type of average value may underpredict early releases.

The diffusion model will consider the two geometries used most widely in LLW disposal: cylindrical (drums) and rectangular (boxes). To simplify the situation, it will be assumed that the concentration in the contacting solution is zero. That is, solution feedback effects are ignored. This assumption leads to the highest predicted release rates and permits an analytical solution to be obtained.

In both models, we analytically solve the diffusion equation corrected for decay.

$$\frac{\partial C}{\partial t} = \Delta \circ D\Delta C - \lambda C$$

where D = the effective diffusion coefficient and all other parameters have been previously defined.

The initial condition assumes a uniform concentration throughout the wasteform:

$$C(x, y, z, 0) = C_o$$

The boundary conditions assume symmetry about the midplane of the wasteform and zero concentration at the outer edge.

$$C(x_b, y, z, t) = 0$$
$$C(x, y_b, z, t) = 0$$
$$C(x, y, z_b, t) = 0$$

where the subscript b denotes a boundary.

Solution of Eqn. (2.13) subject to the initial and boundary conditions gives the concentration at any location within the wasteform. However, the quantity of interest is the release rate, which is the mass flux integrated over the surface area.

$$Q(t) = \int dS \circ J_s$$

where:

Q(t) is the mass release per unit time; and
J_s is the mass flux at the surface.

For one-dimensional diffusion-controlled release,

$$J_s = -D \frac{\partial C(x_s)}{\partial x}$$

where x_s denotes a surface of the wasteform.

Equation (2.13) is solved analytically and used to evaluate the flux as prescribed by Eqn. (2.17). This expression is placed in Eqn. (2.16) and the release rate is determined. The detailed expressions for release rate for both geometries can be found in Appendix A.

2.5.4 Uniform Release Model

The uniform release model assumes that the wasteform release rate decreases in time due only to radioactive decay and solubility constraints. In the Source Term Model Selection report [Sullivan, 1991a] (and in the computer code BLT), this model is named the dissolution model and was meant to represent releases from activated metals which undergo corrosion. Due to the wide variety of waste streams/wasteforms which this model may be used to represent and to avoid confusion with the term dissolution which has a specific definition, the name has been generalized to uniform release model.

In the uniform release model, the release rate is:

$$Q = Q_f M_{wf} e^{-\lambda t} \left[1 - \frac{C}{C_{sat}} \right]$$

where:

Q_f = fractional release rate, and
C = solution concentration at time t.
M_{wf} = initial mass of the contaminant in the wasteform.

and all other variables have been previously defined. Equation (2.18) is analytically integrated over a time step and the resulting expression provides the total mass release in that time step.

The fractional release rate is the fraction of the initial mass in the wasteform that is released per unit time. In the BLT code, the dissolution release model is:

$$Q = \left(\frac{u M_{wf} S}{V_{wf}} \right) \left(1 - \frac{C_s}{C_{sat}} \right) e^{-\lambda t}$$

where u is the dissolution velocity, S is the surface area, and V_w is the volume of the wasteform. Comparing the two expressions, it can be seen that for dissolution release, the fractional release rate is:

$$Q_f = \frac{uS}{V_{wf}}$$

If dissolution release is the appropriate model, Eqn (2.20) can be used to estimate the fractional release rate.

2.5.5 Influence of Localized Failure on Release

If there is localized failure, the intact portion of the container still provides a barrier to release from the wasteform/container system. In this case, the release rates discussed above must be modified to take this into account.

As water enters through the breached area, it might be stored within the container until a bathtub forms and the height of the bathtub reaches the lowest region of failure. At this time, water

would begin to flow out of the container. Accurately predicting the location of failures around a container is beyond the state-of-the-art and will not be attempted here. Instead, it will be assumed that, once a container is breached, there will be steady flow of water into and out of the container. The container flow rate will be the Darcy velocity multiplied by the ratio of the breached area to the total area.

The partially-failed container will be treated as a mixing cell in which radionuclides released from the wasteform are uniformly mixed within the container. The release rate from the container will be the product of the container flow rate and the mixing cell concentration as calculated based on the various release mechanisms. This is identical to the approach used in the BLT computer code [Sullivan, 1989].

2.5.6 Selection of Release Models

As part of this program an evaluation of disposal data has been made [Cowgill, 1992a; Sullivan, 1991; Cowgill, 1992]. These reports discuss the distribution of radioactivity by waste class, waste stream, and wasteform and provide a starting point for selection of the appropriate leaching model.

A major finding of these studies is that in general, there is limited data on releases from most low-level waste streams or wasteforms. The lack of data covers the major waste streams: dry active wastes, dewatered resins, and activated metals. There is substantial data on releases of Cs, Sr, and Co in cement solidified wastes. Unfortunately, only a small fraction of the activity of these radionuclides is in cement. For radionuclides that do exhibit substantial quantities in cement, e.g., C-14, Tc-99, U-238, and Ra-226, there is also limited data.

Due to the lack of data, it is recommended that the surface rinse model be used for all dry active wastes and dewatered resins. If a partition coefficient is available and can be justified it should be used. For cement solidified wastes, leaching data indicate that diffusion controlled release should be used. The choice of diffusion coefficient should be supported by data. If data does not exist, a conservative estimate for the diffusion coefficient is 10^{-6} cm^2/s. This is equivalent to a Leach Index of 6, the minimum allowed by the wasteform technical position [Lohaus, 1991]. For activated metals, a fractional release rate based on typical dissolution rates of the metals may be possible to justify.

For convenience, Table 2.1 presents a summary of the models selected for each of the four processes that influence release from the disposal facility.

2.6 Initial and Boundary Conditions

In both the MCMC and FD transport models, the user must supply the initial concentration at every computational point.

In the MCMC model, boundary conditions are not necessary. The analytical solution assumes that the incoming concentration at the top boundary is zero. The bottom boundary condition is not needed due to the unidirectional flow and the absence of dispersion. That is, the concentration in the last node is independent of processes at the boundary.

In the FD model, both the top and bottom boundary conditions must be defined. One of four conditions are permitted to be specified at each boundary. These conditions are specified: concentration; total flux; advective flux; or dispersive flux. The description of the numerical implementation into the FD equations is presented in Appendix A.

In DUST, boundary conditions are defined through tabular input of the value for the boundary condition at a given time. Interpolation is used to determine the boundary condition value at times not in the table.

The boundary condition of zero concentration leads to the highest releases from the system. This condition implies that processes at the boundary are high enough to remove all material as soon as it exits the system.

The boundary condition of zero total flux prevents mass from leaving the system and causes concentration levels to be at a maximum. This condition is useful at a plane of symmetry or at the top boundary if zero release is desired. The total flux is the sum of the advective flux and the dispersive flux.

The advective flux is the Darcy velocity multiplied by the concentration. The Darcy velocity is known through input, therefore, specifying the advective flux is mathematically equivalent to specifying the concentration. The use of this condition is provided as a convenience to the user.

The dispersive flux is the diffusion/dispersion term multiplied by the concentration gradient. Setting this boundary condition to zero is useful when advection out of the system is the only mechanism for release, for example flow into a lysimeter drain.

Table 2.1 Model Selection Summary

Fluid Flow	Container Failure	Wasteform Release	Transport
Flow rate and moisture content within the disposal facility evaluated using a table look-up.	Each representative container may have different properties, i.e., a) Time to failure. b) Partial failure due to localized effects (e.g., pitting). Early water access. (FD Model)	Each representative wasteform may have different properties. Release characteristics are nuclide specific. Models account for: a) Surface rinse with partitioning (Lab trash, contaminated soils, DAW) b) Diffusion (solidified wastes) - Analytical solutions to the diffusion equation assuming zero boundary concentration (maximum release rate). Release is geometry dependent, models are provided for both cylindrical and rectangular wasteforms. (FD Model) c) Uniform (activated metals) - Constant release rate. d) Solubility limited release. (FD Model)	Transport parameters such as the retardation coefficient are nuclide specific. a) Improved multi-cell mixing cascade models. Mixing cascade models have been generalized to include non-uniform sources, radioactive decay, and non-uniform time-dependent sources with retardation. This model provides an analytical solution for the concentration and is valid for advection dominated flow. b) One-dimensional finite difference model. This model is more appropriate when diffusion and dispersion are important transport parameters. This could occur for gases or for extremely low-infiltration rates.

3. PROCEDURE FOR CALCULATING RELEASES USING DUST

The preceding chapter describes the models selected for estimating the source term but does not provide a clear indication of the steps needed to take the raw data, transform the data into the form required by the models, input the data and estimate the source term. Figure 3.1 is a schematic diagram that outlines this procedure.

The first step in this process is to compile the inventory data for the radionuclides of interest. Three factors that are determined before the waste is emplaced in a disposal facility figure prominently in determining release. These are the radionuclide's waste stream, wasteform, and container. A radionuclide contained in an activated metal will be released at a much different rate than the same radionuclide that exists as a surface contaminant on lab trash. Similar remarks apply for releases from different wasteforms. The container will control the time that release begins and for localized failure, the amount of water that accesses the waste.

Work to determine the feasibility of characterizing the radionuclide inventory based on the three parameters listed above has been done. This effort, based on commercial disposal data from 1987 through 1989 [Roles, 1990], will determine the activity fraction of the waste streams contained in various wasteform and container types (e.g. HIC's, carbon steel, etc.). Discussion of the most important waste stream/wasteform/container systems in terms of activity are provided in [Sullivan, 1991b; Cowgill, 1992; Cowgill, 1992a].

Due to the large number of possible waste stream/wasteform/container combinations it will not be possible, nor even desirable, to model each of these systems individually. Therefore, many of the combinations that do occur should be lumped together to form a "representative" wasteform/container systems. This grouping should be performed to handle the most important wasteforms in terms of release. After the "representative" systems have been identified, appropriate container degradation and wasteform release models and parameters need to be determined.

Using the flexibility of the source term model, it will be possible to specify different release models and parameters for each waste stream/wasteform combination. For example, ion exchange resins solidified in cement may be assumed to follow diffusion-controlled release with one diffusion coefficient while evaporator bottoms solidified in cement may be given another, and activated metals may be assumed to follow dissolution controlled release with a constant release rate. Similarly, for two identical waste stream/wasteforms in two separate containers, the predicted release can be different due to different container properties.

The inventory, container degradation and wasteform release parameters are input into the source term model as schematically depicted in Fig 3.1. These parameters along with the radionuclide specific parameters (e.g. half-life, solubility limit, etc.), transport parameters, water flow parameters (velocity and moisture content), initial conditions, and boundary conditions (finite difference model only) fully describe the problem.

Figure 3.1 Flowchart of the procedure used to take waste stream/wasteform/container inventory data and define the necessary input parameters to estimate the release rate from a disposal facility.

In general, the choice of input parameters used by the DUST code must be justified. Justification can come from experimental data, that is, use measured diffusion coefficients to predict wasteform release, from the use of more sophisticated computer codes, or well-documented expert judgement. For example, the MCMC model in the DUST code assumes a constant flow rate through the disposal unit. In selecting the flow rate, a two-dimensional computer code that predicts unsaturated flow such as VAM2D could be used as a basis for determining this parameter. In any case documentation of the basis for the use of an input variable should be supplied with the results of any simulation. The potential for misusing the simple models through improper choice of input data is large.

Once the data has been selected, an input deck for the DUST code must be created. To facilitate this process, the program DUSTIN was written. DUSTIN is a menu-driven code that prompts the user for the input required by DUST. DUSTIN allows the user to create an entire input deck or, modify an existing input deck. Modifications can be individually made to every single input parameter. Use of DUSTIN is described in Chapter 6.

After creating an input deck, the calculation is ready to proceed. For the MCMC model which relies on an analytical solution, the predicted release is calculated at the times specified through input. For the finite difference model, the predicted release is obtained through solving the differential equation describing release and transport through the disposal facility at a fixed time, incrementing the time and repeating the procedure until the problem is finished.

The output of these models will be the release rate from the disposal unit as a function of time. This output will be stored in tabular form for use with performance assessment codes, such as PAGAN [Chu, 1991], that predict the transport of radionuclides through the unsaturated zone to the aquifer and ultimately to a receptor.

If requested by the code user, DUST creates output files named TRACECND.DAT and TRACEFXD.DAT. These files contain the concentration at specified locations and the flux and mass release at specified locations as a function of time. If the FD transport model is used, the file CONCNT.DAT is written. This file contains the concentration at every location at the times requested in the primary output file. The program GRAFXT.EXE can plot each of these three files on a video display unit. The use of GRAFXT is described in Chapter 9. The procedure to be followed in creating an input deck, running the DUST code and analyzing the output is presented in Figure 3.2.

Figure 3.2 Schematic outline of the procedure used to analyze release from a LLW disposal facility using the DUST code package.

4. APPLICABILITY AND LIMITATIONS OF THE DUST CODE

The DUST code models release and transport of a single radioactive contaminant through a low-level waste disposal facility in one spatial dimension. The source for transport is the contained radioactive wastes emplaced in the facility. Releases are a function of the container performance (time to failure) and wasteform performance (release rate). Each container may be assigned a unique time to failure and wasteform release rate parameters. This permits the flexibility to model a wide range of problems related to a waste disposal facility. These include determining the effects of the following parameters on release from the facility:

a) infiltration (flow rate);
b) container performance;
c) wasteform release rates; and
d) soil transport properties (retardation).

The DUST code can be applied to a wide range of problems pertaining to low-level waste disposal ranging from lysimeter studies in which there is only a single soil and no waste container to below ground vaults with caps, multiple containers and wasteforms, engineered structures and backfill. However, due to the simplifications used in developing the models, the validity of the predicted results depends quite heavily on the input data, as discussed in Chapter 3. Many parameters in DUST (for example, water flow rate and container failure time) are determined within the code directly from user supplied input and not from first principles. Therefore, justification of the choice of input parameters is a critical aspect in developing confidence in DUST predictions.

4.1 Limitations

In developing the DUST code, due to lack of mechanistic data and in order to limit the problem size to make the code executable on small desktop systems within a reasonable time, a number of assumptions were invoked. These assumptions may make use of the code inappropriate under certain conditions. In developing the MCMC model, a number of additional assumptions are used as compared to the FD model. The implication of these assumptions are discussed separately below. A list of the limitations follows.

(1) The DUST code simulates only one spatial dimension. It therefore assumes a uniform geometry in the other two dimensions. This approximation will be best near the center plane of the facility where edge effects are minimized. The lack of spatial resolution may cause problems near special features such as drains or fractures in engineering structures. Modeling the entire facility such that the bottom boundary has the properties of a drain will overestimate release, while modeling the facility as being completely intact may underestimate releases.

(2)The DUST code models flow through a porous medium. Fracture flow, which may become significant at high relative moisture contents, through engineered barriers is not considered.

(3)Water flow and container failure time are not calculated from first principles in DUST. They are determined through input. The user must justify the values used for these parameters.

(4)DUST models only a single species. This influences three major areas: ingrowth due to radioactive decay, production or removal of species due to biodegradation, and interpreting solubility limits.

Ingrowth due to radioactive decay is not modeled. Ad hoc suggestions for modeling ingrowth were provided in the model selection report [Sullivan, 1991a]. For short lived radionuclides in secular equilibrium with the parent, it was recommended that a production term be added to the inventory. In the DUST code, this production term could be included in every container through use of an external source.

Biodegradation can produce radioactive gases, e.g. tritiated methane, $^{14}CO_2$, or $^{14}CH_4$. As a single species code, release in the gaseous and aqueous phase can not be handled simultaneously. An ad hoc procedure which partitions the inventory into the gaseous and aqueous phases may be used provided the code is run twice, once with the appropriate inventories and flow parameters for gaseous release and once for aqueous release. Work on estimating the partitioning between the gaseous and aqueous phases has been recently initiated.

In modeling only a single nuclide, care must be taken to insure that solubility limits are not exceeded if other species containing that element exist. The solubility limit used in the DUST code applies to the modeled nuclide only. If the element exists in more than one nuclide, the solubility limit must be decreased to account for this problem. For example, if the DUST code were used to model U-238 and solubility limits are used, this solubility limit should reflect the presence of other uranium species.

(5)DUST does not model changes in chemistry. The chemistry of the disposal facility is modeled through the distribution coefficient. Changes in this parameter due to changes in pH, Eh and competition with other ions for sorption sites are not considered.

(6)In the FD model, the diffusion release subroutine is independent of the concentration in solution and solubility limits. This is a result of using the analytical solution based on a boundary condition of zero concentration at the wasteform-solute interface.

(7)In the MCMC model, the Darcy velocity must remain constant at all times. In the FD model, the Darcy velocity is calculated from a table of velocity versus time.

(8)In the MCMC model localized container failure is not modeled.

(9)In the MCMC model the distribution coefficient and moisture content must be constant throughout the facility and in time. The FD model permits these parameters to vary spatially.

(10) In the MCMC model release mechanisms are limited to the uniform release and rinse release without a wasteform partitioning factor. The FD model allows a partitioning factor and models diffusion controlled release.

(11) As shown in the development of the equations, both the MCMC and FD models use upwind differencing to model the advection term. Upwind differencing insures that information is only advected downstream, however, it leads to numerical dispersion. The value of the numerical dispersion coefficient, D_n, in the FD model is [Roache, 1976]:

$$D_n = \frac{V_d \Delta x}{2}(1 - C)$$

where V_d is the Darcy velocity, Δx is the size of the finite difference node, C is the dimensionless Courant number, $V_d \Delta t / \Delta x$, and Δt is the time step size. In the limit as the time step size approaches 0, the solution to the FD equation approaches the solution of the original differential equation modified due to numerical dispersion. In this case, the Courant number goes to zero and the numerical dispersion coefficient becomes:

$$D_n = \frac{V_d \Delta x}{2}$$

Heuristically, this can be viewed as the numerical dispersion coefficient for the MCMC model which uses an analytical solution. Numerical studies comparing the FD model with zero mechanical dispersion and diffusion with the MCMC model support this heuristic estimate of numerical dispersion for the MCMC model.

Recalling that the mechanical dispersion term from Eqn (2.1) is:

$$D = V_d \, a_l ,$$

it is seen that the numerical dispersivity is $\Delta x/2$. Therefore, if the mesh size is more than twice as large is the mechanical dispersivity value, numerical dispersion will dominate. From the numerical dispersion expression it is clear that it can be minimized through taking small nodes. As a rule of thumb, the mechanical dispersion is typically 1/10 to 1/100 of the scale of the modeled domain. Therefore, Δx should be much smaller than 1/5 to 1/50 of the modeled domain to insure that numerical dispersion is unimportant.

(12) Although conceptually, modeling gas flow through the facility is similar to modeling water flow, there is extremely little data on production of radioactive gases or expected flow rates. Therefore, the user must be extremely careful when selecting these values.

Radionuclides disposed of in gaseous form are expected to release quickly after container failure. For adsorbing gases it is expected that release would be controlled by a partitioning factor. Gases can also be formed by biodegradation, for example, tritiated methane, $^{14}CO_2$, or in the case of radon, through radioactive decay of radium. Few data exists on the formation of radioactive gases in a disposal facility. However, tritiated methane, $^{14}CO_2$, ^{14}CO, and other radioactive gases have been detected at the closed disposal sites at Sheffield [Streigel, 1985] and West Valley [Kunz, 1982; Matuszek, 1983]. While it is likely that the better disposal techniques (concrete vaults, no wooden or cardboard containers, solidification of the wastes in cement, etc.) planned for the new facilities may lead to less organic material, many of the wastes contain significant amounts of organics. This is particularly true for ^{14}C wastes [Gruhlke, 1986]. Therefore, releases caused by biodegradation cannot be dismissed at this time.

As a final caveat, uncertainties in the input data are often the most significant limitation in many models and codes. Frequently, many input parameters are not accurately known or available. Users of the DUST code should be constantly aware of the limitation imposed by the quality of the input data.

5. VERIFICATION TESTS

A number of studies have been conducted to verify that the computer code, DUST, correctly calculates the properties of interest (time of container breach, wasteform release rates, solution concentration, and mass flux). Independent testing of the container degradation models (general and local failure) and the wasteform release models (diffusion, uniform, surface rinse with partitioning, and solubility limited) was performed for problems with known analytical solutions.

The FD and MCMC transport models received extensive testing through comparison of predicted results to analytical solutions and through comparison of the MCMC results and FD results on identical problems.

For verification testing, Eqn (2.3) has been solved for a semi-infinite medium and the following initial and boundary conditions:

$$C(x,0) = C_i$$

The boundary condition at x = 0 is:

$$\left(-\theta D \frac{\partial C}{\partial x} + V_d C \right) = \begin{cases} V_d C & 0 < t \le t_o \\ 0 & t > t_o \end{cases}$$

where C_o and C_i are constant. The analytical solution to this problem is presented in [Van Genuchten, 1978].

The analytical solution requires a non-zero value for the diffusion/dispersion term. Therefore, the FD model was tested against the analytical solution for three problems. In these problems, advection, dispersion, retardation, and decay are modeled. Three test cases were run. In these cases, the parameters chosen for the model were selected to correspond to the values used by Van Genuchten and can be found in Table 5.1.

Table 5.1 Parameters used to verify the finite difference transport model

	Case 1	Case 2	Case 3
Darcy Velocity (cm/s)	2.89E-4	2.89E-4	2.89E-4
Dispersion/Diffusion (cm^2/s)	4.34E-4	4.34E-4	4.34E-4
Decay constant (1/s)	2.51E-6	0.0	2.51E-6
Source (curies/(cm^3-s))	0.0	0.0	1.16E-5
Moisture content	0.3	0.3	0.3
Retardation coefficient	3.3	3.3	3.3

The semi-infinite domain was modeled using 300 cm. and comparing the semi-infinite analytical solution to the numerical solution over the first 100 cm. for the first 10 days. Numerical studies were performed with the DUST code to show that, for this time frame and distance, the boundary conditions at the 300 cm. boundary do not influence the results.

In the first problem, case 1, solute was injected into the boundary at $x = 0$ for 5 days such that the incoming concentration was 1 Ci/cm^3. After the fifth day, the flux at $x = 0$ is zero. At the boundary away from the injection source, the boundary concentration is set to zero. The initial condition is zero concentration throughout the modeled domain. Advection, dispersion, retardation and radioactive decay were modeled.

Figure 5.1 presents a comparison of the analytical and numerical solution predicted by the DUST code at 5 and 10 days. The agreement between the two is excellent. The maximum difference between the two solutions is less than 2%.

Test case 2 was identical to case 1 with the exception that the decay term was set to zero. This is a slightly more difficult numerical problem because the concentration gradients are larger than in case 1. Again, the agreement between the analytical and numerical solutions at 5 and 10 days is excellent, Figure 5.2.

Test case 3 has the same transport properties as test case 1, Table 5.1, however, the problem begins with a uniform initial concentration of 10 Ci/cm^3, a uniform source of 1.16E-5 $Ci/cm^3/s$, and zero total flux at the x=0 boundary. This problem tests the proper use of the external source (i.e., wasteform release) term and use of non-zero initial conditions.

Figure 5.3 contains a plot of concentration versus distance at 2, 5, and 10 days. The results indicate that the DUST code is capable of reproducing the analytical solution with a high degree of accuracy.

Figure 5.1 Test case 1, comparison of the DUST finite difference model predictions with the analytical solution for a pulse source at x=0 for 5 days. Retardation and decay are modeled. See Table 5.1 for the model parameters.

Figure 5.2 Test case 2, comparison of the DUST finite difference model predictions with the analytical solution for a pulse source at x=0 for 5 days. The decay term is zero in this simulation. See Table 5.1 for the model parameters.

Figure 5.3 Test case 3, comparison of the DUST finite difference model predictions with the analytical solution for a uniform initial concentration, zero total flux at the boundary x=0, and an external uniform source. See Table 5.1 for the model parameters.

In the preceding problems, diffusion/dispersion plays an important role in the transport of the radionuclide and therefore, the analytical mixing-cell cascade model cannot be used. The mixing-cell cascade model was compared directly with hand calculations of the analytical solution [Appendix A] for several simple problems (few cells, all containers fail simultaneously, constant release rates). In addition, a number of test cases were run in which the diffusion/dispersion term was set to zero in the FD model. This allowed comparison of the predictions of the FD and MCMC models directly.

Test case 4 is an example of one of these problems. In test case 4, the domain for the finite difference model is 50 meters. For this simulation, the domain was subdivided into 50 regions, each 1 meter in length. The first 10 meters contain only soil. In the next 24 meters there is a wasteform every other meter for a total of twelve wasteforms. The container failure times range from 0 to 40 years as presented in Table 5.2. Release from the wasteforms is modeled using the uniform release model. The parameters for this model were chosen such that once water contacts the wasteform the fractional release rate is 5% per year, all other parameters are presented in Table 5.2. The problem considers radioactive decay, retardation, and advection.

Table 5.2 Parameters used in test case 4: Comparison of the mixing cell and finite difference model results

Container failure times:

Location (m)	1	3	5	7	9	11	13	15	17	19	21	23	
Time (yrs)		0	10	20	30	40	0	10	10	20	20	0	30

Release and Transport Parameters:

Darcy Velocity (cm/s):	1.59E-6
Moisture Content:	0.2
Retardation coefficient	9.0
Release rate (1/yr)	0.05
Half-Life (yrs)	12.33

The mixing cell simulation was identical to the finite difference model with the exception that only 40 meters was modeled. For advection driven flow, the 10 meters upstream from the wasteform do not receive any contaminant. Thus, the two test cases are identical except that the distance from the top of the simulation domain is offset by 10 meters. The difference is necessary to insure that the boundary condition of the finite difference solution does not influence the results.

Figure 5.4 presents a comparison of the results of the two simulation techniques at three different locations for a 90 year period. Location 1 is 7 meters from the top of the first wasteform, this cell has a container that fails after 30 years. Location 2 is 12 meters from the top of the first wasteform. It does not contain a wasteform. However, the adjacent upstream cell has a waste container that fails instantly. Location 3 is 23 meters from the top of the first wasteform. It has a container that fails after 30 years. Two meters upstream from this wasteform is a waste container that fails instantly.

In all locations and at all times, the mixing-cell model and the finite difference model show excellent agreement. At location 1, x = 7 m in Fig. 5.4, there is a gradual buildup of the concentration in time due to container failures upstream. At 30 years, there is a slight jump in concentration due to the failure of the container in the cell. At location 2, x = 12 m in Fig. 5.4, there is a rapid rise in concentration at early times due to the failure of the container 1 meter upstream. The concentration peaks after about 10 years and begins to decline for approximately 30 years. At this time, other containers upstream have failed and begun to release contaminants. The concentration shows a local maximum after about 50 years as the containers 3 and 5 meters upstream failed after 40 and 30 years, respectively. At location 3, x = 23 m in Fig. 5.4, there is a peak after 12 years due to failure of the container 2 m upstream at emplacement. The concentration decreases until 30 years where a sharp increase occurs due to the failure of the container in this cell.

Figure 5.4 Test case 4, comparison of the DUST finite difference and mixing cell cascade model at three locations. There are 12 wasteforms, each one meter in length separated by one meter of soil beginning at x=0. The container failure time differs for the wasteforms as described in Table 5.2. Release and transport parameters can also be found in Table 5.2

6. DUSTIN: A PREPROCESSOR THAT CREATES AN INPUT DECK FOR DUST

In order to facilitate ease of use of the DUST computer code, a pre-processor which takes the user through all of the steps necessary to create an input deck has been written. This pre-processor, DUSTIN, relieves the code user of knowing the exact format and structure of an input deck and is menu driven. The menus present a series of choices and generally request a numeric response. In the few cases when an alpha-numeric response is required, e.g., defining titles, this is clearly noted.

DUSTIN has the flexibility to independently alter any single parameter required by the DUST code. DUSTIN has the capability of creating an entirely new input deck or reading a partially or fully completed input deck which can then be modified. A major advantage in using the DUSTIN code is that it provides an annotated input file for DUST. This greatly facilitates direct modification of the input deck, Chapter 7.

The first menu asks the user if a completely new input deck is to be created or if an existing input deck is to be modified. After this decision has been made, the code proceeds to the main menu. The main menu permits the user to modify any variable required for input to the DUST code independently through access to sub-menus. After the input variables have been defined, DUSTIN allows the user to create a trial input deck or create a "partial" input deck. The flexibility allowed in being able to independently modify any single variable within the code makes it nearly impossible to guarantee that a consistent input deck is created by the DUSTIN user. Although, there are many checks within the code to prevent obvious problems, it is possible to create an invalid input deck. For example, the user could define the number of containers to be 20 and not specify any failure parameters for the containers. If this occurs, DUSTIN will try to make an input deck if requested, but obviously the input deck will not be valid. For this reason, DUSTIN permits the user to create an output file that is identical to the output file that would be obtained if the DUST code were used. This is a useful aid in debugging the trial input deck.

In addition, DUSTIN permits the user to create a "partial" input deck which can be read in later by the DUSTIN code and modified as necessary. Use of this feature is strongly recommended. A "partial" input deck is any set of input data created by DUSTIN using the namelist procedure described later in this section. The advantage to this approach is that the check to determine if the data forms a valid input file is not made when reading the data. In contrast, if the user attempts to read in a completed input deck that is not valid, an error message is printed and control is returned to the operating system. That is, data on an invalid completed input deck cannot be modified by DUSTIN.

The remainder of this chapter takes the reader through the various menus that appear when running the DUSTIN computer code. All sections that have a double border and are highlighted in boldface print are the screens that appear on the console. Italic characters are examples of the code users response to the query. For convenience in referencing and to enhance the ease of locating discussions of the parameters, the numbering system for this chapter will correlate to the numbers in the main and secondary menus. For example, Section 6.4.3 will refer to the fourth item on the

main menu and the third item on the secondary menu. For this reason, the input selections menu and the main menu will appear in this section.

In general, far fewer variables are needed to use the Multi-cell Mixing Cascade (MCMC) transport model as compared to the Finite Difference (FD) transport model. These differences are explicitly and prominently mentioned in the DUSTIN code. For example, if the user attempts to define a variable that is not required by the MCMC model, the DUSTIN code will print a message indicating such. If a variable is required by only one model, the designator FD or MCMC will be displayed at the top of the section describing the variable.

This chapter will serve as the most detailed reference on the input variables required for DUST. In addition to describing the operation of the DUSTIN code, selection of the appropriate values for the physical parameters, instructions on the operations of the models, and recommendations on when to use certain models will be primarily provided in this chapter.

INPUT SELECTIONS:

When running the DUSTIN code, the first menu is:

```
                Input selections

1)  Input data for new input deck
2)  Read stored data from BLOKxxx file
3)  Modify/Inspect existing input deck
```

Choice = 1:

The code user will create an entirely new input deck. Default values are specified for some parameters but generally these need to be redefined. After choosing this value, the main menu is displayed.

Choice = 2:

Upon entering a value of 2, the following screen is displayed:

```
Enter 3-digit NUMERIC code of existing BLOKxxx file:
Enter choice: 1 (user input)
```

```
File BLOK001 is being accessed;
STANDBY

 1 = Go to MAIN MENU
 2 = Create input deck and see OUTPUT file
Enter choice:
```

DUSTIN will read a file previously prepared by DUSTIN called BLOKxxx, where xxx is a three digit number. In the example, the 1 digit number is translated by the code to 001 and the file BLOK001 is read. BLOKxxx is a file created by using FORTRAN namelists. As such, it is an exact copy of all the input variables needed by the DUST code at the time that the file was written. There are no checks on whether this set of variables forms a valid input deck. Therefore, the BLOKxxx file is useful when the code user is uncertain if a valid input deck has been created or if a partial input deck has been created.

The code checks to determine if the BLOKxxx file exists. If it does not exist, the user is returned to the Input Selections Menu. After successfully reading the file, the code user is allowed to attempt to make an input deck or proceed to the main menu.

Choice = 3:

The code requests the name of the input file, a name for the output file to be created, and if the output file exists, the code asks if the file should be overwritten. The completed screen for this procedure is displayed:

```
Enter the path\name.extension for the DUST input file
created by this program:   case8-9a.inp

Enter the path\name.extension for the file that this
code creates as a check on the input:   case8-9a.out


Error code = 70
The file you have specified already exists -
Do you wish to overwrite this file (0 = No, 1 = Yes)
Enter choice: 1
```

The DUSTIN code then proceeds to the Main Menu. If the file case8-9a.inp did not exist or if the file does not contain a valid input deck, the code fails and control is returned to the operating system.

MAIN MENU:

The main menu consists of a list of general categories that comprise the groups of input parameters needed by the DUST code. The main menu provides access to the sub-menus defined by the grouping scheme. Definition of the input variables occurs in the sub-menus. This section will provide a description of the main menu and the variables contained under the grouping scheme. Detailed discussions on the variables and how they impinge on model predictions will be presented when discussing the sub-menus. The main menu for DUSTIN follows:

```
                    MAIN MENU

1)  General problem definition
2)  Time parameters
3)  Material assignments/properties
4)  OUTPUT specifications
5)  Facility dimensions and coordinates
6)  Initial and boundary conditions
7)  Water flow and moisture content
8)  Container parameters
9)  Wasteform parameters
10) Source/Sink parameters
11) Create input deck for the DUST code
12) Store partial input in BLOKxxx file
13) Exit program without saving data

Enter choice:
```

Choice = 1: General problem definition

The general problem definition includes variables which define the following: title, name of the radionuclide, half-life, atomic mass, solubility limit, a flag to specify if the input is in mass units of grams or curies (if the input is in curies, the code internally translates this to grams for consistency with the units on the distribution coefficient and solubility limits, upon output, the mass is translated back into the original input units), number of control volumes or mixing cells in the computation, and the flag for selecting the multi-cell mixing cascade or the finite difference transport model.

Choice = 2: Time parameters

Time parameters include the number of output times and their values for the MCMC transport model and the number of time steps, the number of time step changes, the initial time step, fractional change in time step, maximum time step, and maximum problem time for the FD transport model.

Choice = 3: Material assignments/properties

Material properties for the MCMC model include the bulk density and soil distribution coefficient. The MCMC allows only one material type. The FD allows multiple material types and requires the number of materials, the material type for each control volume, the bulk density and the soil distribution, dispersion, and diffusion coefficients.

Choice = 4: OUTPUT specifications

Output specifications include printer control variables which determine if output occurs at each time step, the number and location of concentration and flux traces, and the number of time steps between writing values to the trace files.

Choice = 5: Facility dimensions and coordinates

Facility dimensions and nodal coordinates include the surface area and height of the facility for the MCMC transport model. The MCMC model assumes uniform spacing and, therefore, the thickness of each cell is the height of the facility divided by the number of cells. The FD transport model allows variable thickness cells and, therefore, the thickness of each cell must be specified along with the facility surface area. The height of the facility is calculated from the input when the FD transport model is specified. The surface area of the facility is a normalizing factor to account for the volume of the 3-D facility in a 1-D model. It is an important parameter in determining concentrations of radionuclides in solution. For example, if the mass inventory is released instantly and uniformly across the facility, the concentration is determined from the inventory, height, surface area, and moisture content. Since dose is proportional to concentration, the normalization by surface area is required.

Choice = 6: Initial and boundary conditions

Initial and boundary conditions are required for the FD model. The boundary conditions for the MCMC model are fixed (zero incoming concentration) by the analytical solution of the model and are not required. The FD model allows specified concentration, total flux, advective flux, or dispersive flux as a boundary condition.

Choice = 7: Water flow and moisture content

The Darcy velocity and moisture content are required by both transport models. The MCMC model permits only a time-invariant uniform Darcy velocity and moisture content in the modeled domain. The FD model permits a spatially uniform, time-varying Darcy velocity, and a spatially varying, time invariant moisture content. A time varying Darcy velocity could be used to model degradation in the ability of the cap to prevent water ingress.

Choice = 8: Container parameters

Container parameters in the MCMC model include the number of containers, their location in the modeled domain and their failure time. In addition, the FD model allows localized (pitting) failure and, therefore, requires information on the localized failure rate parameters as well as assignment of these parameters to each container.

Choice = 9: Wasteform parameters

Wasteform release parameters include the inventory, the number of different sets of release rate parameters, a flag to indicate which release rate parameters are to be used on each waste form, and the release rate parameters. The MCMC model permits only rinse release subject to partitioning and an exponentially decaying release rate where the exponent accounts for radioactive decay. In addition, the FD model permits diffusion controlled release from either cylindrical or rectangular finite sized waste forms. Therefore, input is required to define the diffusion coefficients and the dimensions of the waste form.

Choice = 10: Source/Sink parameters (FD Model Only)

In addition to the waste forms releasing contaminants into the system, external sources or sinks can be specified by the code user if the FD transport model is specified. These sources are defined through tabular input which provides the source strength as a function of time, as well as input specifying the number of sources, the number of different types of sources (e.g., number of source strength versus time tables), the location of the sources, and the assignment of a source type to a location.

Choice = 11: Create input deck for the DUST code

This selection creates the input deck to be used by the computer code DUST. It first asks for the file name for the input file. If it exists, it asks the user if it should overwrite this file. It then asks if an attempt to create an output file should be made. If so, it requests the name of the output file. After completing this task, control is returned to the Main Menu. This can be useful when creating multiple decks in which only a few parameters change.

Choice = 12: Store partial input in BLOKxxx file

This option writes the file BLOKxxx where the values for xxx are determined through input. After completing this task, control is returned to the Main Menu.

Choice = 13: Exit program without saving data

Selection of this value exits the program. Control is returned to the operating system.

6.1 General Problem Definitions

```
                    General problem definitions

1)  Problem title ( < 60 characters):
          XXXXXXXXXXXXXXXXXXXX
2)  Radionuclide:  XXXXXXX
    Half-life (yrs) of XXXXXXX. . . . . .          0.00000E+00
    Atomic mass of XXXXXXX. . . . . .              0.00000E+00
    Solubility limit of XXXXXXX . . . . . .        0.00000E+00
3)  Mass flag (10 = grams, 1 = curies). . . . . .             0
4)  No. of Nodal Points / Mixing Cells. . . . . .             0
5)  Transport flag (0 = Mix.Bath, 1 = Finite Diff).           0
6)  Exit to MAIN MENU

Enter choice:
```

On every sub-menu the most recent values for the various parameters are printed when the menu is accessed. The XXXX values for alpha-numeric characters indicate input has not been specified. In this example, the user is creating a new deck and nothing has been specified. If the user had read in an existing input file, the values would be those found in that file.

6.1.1 Problem Title

An alpha-numeric string up to 60 characters in length that describes the problem. Use of the character "/" causes problems when creating BLOKxxx files because the namelist procedure takes this as a variable delimiter. Therefore, use of "/" is not recommended.

6.1.2 Radionuclide

DUSTIN has an auxiliary file called RNUCL.DAT that contains over 200 radionuclides, their half-life in years, atomic mass, and a default solubility limit of 10 gm/cm^3. The atomic mass is used when converting mass between curies and grams. The solubility limit is used in controlling release. It is well known that solubility values are highly dependent on the environment. The default value has been selected to be large enough that solubility limits will not influence release. If better values for this number are defensible, they can be input to the code. When choice 2 is selected, the following menu is displayed:

```
Enter choice: 2
Enter radionuclide name using capital letters
e.g., Cesium-137 is input as CS-137:  SR-90
```

```
Current values for the radionuclide SR-90
  1) Half-life (yrs)                    29.0000000000000
  2) Atomic Mass                        90.0000000000000
  3) Solubility limit (gm/cm**3)        10.0000000000000

If you wish to change one of these parameters
enter the appropriate number (1, 2, or 3)
or enter 0 for no further changes
Enter choice: 0
```

Capital letters are required for the radionuclide name because the computer code takes the input name and performs a string comparison with the radionuclides on the file RNUCL.DAT. If the radionuclide name does not match any of those on file, the code allows the user to either try another name, or enter the values for half-life, atomic mass and solubility limit.

6.1.3 Units Flag for Mass Input

Mass can be input in units of curies or grams. If the input is in curies, the code uses the half-life and atomic mass to convert to units of grams. This is done for consistency with Kd values, wasteform partition coefficients, and solubility limits. For user convenience all output is converted back to the original input units. That is, if the input is in curies, the output is in curies.

6.1.4 Number of Computational Cells

The number of nodal points (FD method) or mixing cells (MCMC method) are input. Currently, the maximum value is dimensioned at 500.

6.1.5 Transport Flag

Flag that selects the method of solution for the transport equation. Enter a value of 1 for the finite difference method. The MCMC method is the default.

6.2 Time Parameters

```
                        Time parameters

1)  No. of time intervals (FD Model Only). . . . . .          0
2)  Number of output (Mix Cell Model) or DELT changes. . .    0
3)  Time(s) of output/DELT changes

    The following are required only by the Fin Dif Mod.

4)  Initial time interval value (DELT-Fin. Dif Mod).    0.00000E+00
5)  Fractional change in DELT at each time step. . .    0.00000E+00
6)  Maximum value of DELT (yrs). . . . . .              0.00000E+00
7)  Maximum simulation time (yrs). . . . . .            1.00000E+03
8)  Exit to MAIN MENU

Enter choice:
```

6.2.1 Time Intervals (FD)

The maximum number of time steps permitted in solution of the finite difference transport equations. Maximum value is 1000. Unused in the MCMC model.

6.2.2 Number of Output (MCMC) or Time Step Changes (FD)

This input variable, (NDTCHG within the code), serves a dual role depending on the choice of transport model. If the MCMC model is selected, the user must supply the number of times at which a calculation is performed.

If the FD model is selected, the time step size is determined from the initial time step and a multiplier applied at the end of each time step. The size of the time step is limited by a maximum value of the time step, (DELMAX). For example, if the time step is 1, and the fractional multiplier is 0.1. The second time step is 1.1, the third is 1.21, etc. The increase is applied until the maximum value is reached, Sections 6.2.4 - 6.2.7. Time step logic within the code permits the time step to be reset to the initial time step at user specified times. This can be useful if it is known a priori that an event that will change the movement of contaminants will occur at a specific time. For example, if it is known that containers fail at 20 and 50 years, the user may want to have relatively small time steps around the times of container failure. This can be achieved through resetting the time step at these two times.

6.2.3 Output Times or Time Step Changes

In the sub-menu, it should be noted that a value is not listed for this parameter. This occurs because this parameter requires an array of values. Upon selection of this sub-menu item, the current values in the array are printed. All parameters that require an array are presented in this fashion.

Again, this is a dual role variable. For the MCMC model this input specifies the times (in years) at which output is requested, with one value for each output time requested in 6.2.2.

For the FD model, this input specifies the time at which the time step is to be reset to its initial value. If this value is greater than the maximum problem time, the time step is never reset.

6.2.4 Initial Time Step (FD)

Initial time step size in years.

6.2.5 Fractional Time Step (FD)

The fractional change in time step is input in this section. Assuming that the maximum time step has not been reached and the time step has not been reset, the time step size at the N-th calculation is:

$$DT_N = DT_i * (1 + FRX)^{(N-1)}$$

where DT_N = the N-th time step.
DT_i = initial time step, and
FRX = fractional change in time step.

At the time at which the time step is reset to its initial value, the value of N is reset to 0.

6.2.6 Maximum Time Step (FD)

Maximum value for the time step (years). This value should be selected based on the problem being modeled and the degree of accuracy required in the solution.

Although the solution procedure used is fully implicit, as a rule of thumb, the contaminant should not move more than the width of a computational cell in one time step. Therefore, the following relationship should be maintained:

$$\frac{V_D \Delta t}{R \Delta x} < 1.0$$

where V_D is the Darcy Velocity, Δt is the time step size, R is the retardation coefficient and Δx is the cell width. The above expression can be used to obtain a maximum time step.

6.2.7 Maximum Simulation Time (FD)

Maximum problem time (years), the default value is 1000 years. In the MCMC model, this is automatically set to the last value for the output time.

6.3 Material Assignments/Properties

If the MCMC model has been selected, the analytical solution permits only one material type in the facility. Therefore, the DUSTIN code does not permit the user to redefine material types and sends the user to the material property definition menu. The following screen appears in this case.

```
Transport flag = 0 : MIXING CELL MODEL specified.

This model assumes that only ONE material type exists.
All nodes are thus assigned material type 1


Material properties:
0)    Exit (keep these values)
1)    Distribution coefficient.....0.000000000000000
2)    Bulk density.................0.000000000000000
3)    Enter both properties


Enter choice:
```

The user can then modify the two material properties used in the MCMC model, the distribution coefficient (cm^3/gm) and the soil bulk density (gm/cm^3). These values are used to calculate the retardation coefficient.

If the FD transport model is used, up to 10 different material types can be specified throughout the facility. This additional flexibility requires that each control volume is assigned a material type. The code automatically defines all control volumes as material type 1. Therefore, definition of material type is required only for control volumes that are not material type 1. The FD model material properties menu is:

```
                    Material properties

 1)  No. of different materials (FD) ..................... 0
```

```
2)  No. of changes to material type assignments (FD) ... 0
3)  Properties of each material type
4)  Exit to MAIN MENU
```

6.3.1 Number of Different Materials

The variable specifies the number of different materials in the facility. The maximum value is 10.

6.3.2 Material Type Assignments

Material type reassignment is achieved through the following routine. Explicit instructions and variable definitions are provided when running DUSTIN as in the example that follows.

In this example, the code asks for the number of material type reassignments. To minimize input errors, the DUSTIN code uses a routine that requires the user to input values within a specified range. The maximum and minimum of the range are determined internally by the code and are based on consistency with previously defined values. In this example, the maximum value of 100 is determined as the maximum number of control volumes as specified in Menu 1.4.

In this case, the code user asked to reassign 10 nodes (control volumes). The code then prints the instructions and definitions for the input variables. The first of which is the node number for the first node in this sequence. Again, Min and Max values are calculated by the code. The user selected a value of 90.

The code asks for the number of nodes to be reassigned in this sequence. The user requested 10, the total number previously specified. If the first node in the sequence was 95, the code would permit only 6 nodes (nodes 95 - 100 inclusive) to be redefined. For the increment between nodes, the code calculated that the maximum increment was 1 and forces the code user to input a value of 1. If for example, the user asked to redefine 2 nodes starting at node 90, the maximum increment would be 10 (i.e., nodes 90 and 100 could be defined on this card) and any value between 1 and 10 would be acceptable.

The code asks for the material type to assign to the first node in this sequence. The maximum value of 3 was determined from the value specified in Menu 3.1. The code user selected material type 3.

The increment in material type to each node was determined to be zero (there are only 3 materials). In a 1-D simulation most often, the materials will occur in layers covering several nodes and zero will be the appropriate choice. However, if the material types change in a regular fashion, this feature may be used.

Upon completing this sequence of input, the code prints out the values and asks if they are acceptable. In the example, we have defined nodes 90 - 99 to be material type 3. Note, node number 100 is still material type 1.

```
No. of material corrections (MIN=0,MAX=100):
(Number of nodes whose material type assignments
 will NOT have the default value of 1)
Enter choice: 10

Material type re-assignment is achieved through a
sequence of five integer numbers.  These numbers are:

1) The location (node #) of the first node in the seq.
2) The number of nodes to be reassigned.
3) The increment of the nodes in this sequence.
4) The material type for the first node in the seq.
5) The increment of material type for the nodes in the seq.

For example, to assign even number nodes between 10 - 24
to have material type 2 use the following values:
1) = 10:       2) = (24-10)/2+1 = 8:
3) = 2:        4) = 2:                    5) = 0

Node # of the first node of sequence 1
to be re-assigned: (MIN=1,MAX=100)
Enter choice: 90

No. of nodes that will be re-assigned in this
sequence: (MIN = 1,  MAX = 10)
Enter choice: 10

Increment of nodes that will be re-assigned:
 (MIN = 1  MAX = 1)
Enter choice: 1

Material type of first node in sequence 1:
 (MIN = 1,  MAX = 3)
Enter choice: 3

Increment of the material type index for the
subsequent nodes in the sequence: (Normally this
would be zero, i.e., all nodes in the sequence belong
to the same material type.  It is non-zero if they
change in a linear manner.)
 (MIN = 0,  MAX = 0)
Enter choice: 0

Values for this card (sequence) are:

  First  Number   Increment    Material    Increment
```

```
 Node     in Seq      Node          Type       Mat'l Type
  90        10         1             3             0

0 = Re-enter THIS sequence
1 = Continue
Enter choice: 1

Material type re-assignment complete.

 First   Number    Increment     Material     Increment
 Node    in Seq      Node         Type       Mat'l Type
  90       10         1            3             0

Press Enter to Continue.
```

The code checks to determine if the number of material type reassignments equals the total number specified in Menu 3.1, if it does, the sequence of numbers that define material type are printed. If it does not, the code returns to the beginning of this section and asks for more reassignments. Although there is a check on the total number of reassignments, there is no check on whether a node has been reassigned twice. For example, the user could specify that nodes 1 - 5 are material type 2 in the first sequence and then specify nodes 3 - 7 are material type 3 in the second sequence. The code would then only define 7 nodes having material properties different than material 1.

6.3.3 Material Properties

For the FD model, four soil material properties (distribution coefficient, bulk density, dispersivity, and diffusion coefficient) are required. The following example provides a typical input session for the first material. First, the code prints out the existing values for all material types (specified in Menu 3.1). If the user decides to change some of these properties, the code asks for the material type to change, prints out the existing values for that material and allows the user to change any one of the values independently or all of the values simultaneously. In this example, all of the values are changed. The units required for the various parameters are printed to remind the user that cgs units are used for material properties. After the user has input the parameters, the code prints these values and allows the user another chance to change the input. If the input is correct, the code returns to the materials properties menu and asks for changes in other materials.

```
                    Material properties:

                                        1           2           3
Material
Distribution coefficient.....    0.00E+00    0.00E+00    0.00E+00
```

```
Bulk density.................   0.00E+00   0.00E+00   0.00E+00
Dispersivity.................   0.00E+00   0.00E+00   0.00E+00
Diffusion coefficient........   0.00E+00   0.00E+00   0.00E+00

0 = Done with material properties
1 = Change material properties
Enter choice: 1

Enter the material type to be changed:
  (Min = 1, Max = 3)
Enter choice: 1

Values for material type 1:
0)   Exit (keep these values)
1)   Distribution coefficient.............0.000000000000000
2)   Bulk density.........................0.000000000000000
3)   Dispersivity........................0.000000000000000
4)   Diffusion coefficient................0.000000000000000
5)   Change all properties
Enter choice: 5

Enter distribution coefficient, in cm3/gm: 1.5

Enter bulk density, in gm/cm3: 1.4

Enter dispersivity, in cm: 25.0

Enter diffusion coefficient, in cm2/sec: 1e-6


Values for material type 1:
0)   Exit (keep these values)
1)   Distribution coefficient.............1.5000000000000
2)   Bulk density.........................1.4000000000000
3)   Dispersivity........................25.0000000000000
4)   Diffusion coefficient...............0.10000000D-005
5)   Change all properties
Enter choice:
```

6.4 Output Specifications

This sub-menu controls output produced by the DUST code.

```
                OUTPUT specifications

1)  Printer control parameters
2)  No. of concentration traces ..............  0
3)  Location(s) of concentration traces
4)  No. of flux traces .......................  0
5)  Location(s) of flux traces
6)  No. of time steps between traces .........  1
7)  Exit to MAIN MENU

Enter choice:
```

6.4.1 Printer Control Parameters

The first menu item controls the main print out. In DUST there is a variable KPR(I) where I ranges from 1 to the number of time steps in the FD model and to the number of output times in the MCMC model.

For the FD model, if KPR(I) = 0, nothing is printed at the I-th time step. If KPR(I) = 1, the concentration at each finite difference point is printed. If KPR(I) = 2, the concentration and flux are printed. If KPR(I) = 3, container breach and wasteform release parameters are printed. When using the FD model, often many intermediate calculations are performed to enhance numerical accuracy, therefore, zero is the default value for all items in KPR. Thus, in order to obtain the main output, some of the values for KPR must be specified. At every time step in which KPR > 0, the concentrations at every location are written to the file CONCNT.DAT. This file can be used by the program GRAFXT to graph the data on the video console.

For the MCMC model, output is slightly different. In the MCMC model predictions are obtained from an analytical solution which is calculated only at the times and locations specified through input. The times for output are specified in Menu 2.3 and the locations are specified through the trace files, Menu 4.3 below. Again KPR(I) = 0 prints nothing. However, KPR(I) = 1 prints the concentration and fluxes at the trace locations specified. The MCMC model does not have any temporal output pertaining to release from the wasteform or container breach. In this model, container breach is specified via input as the time to failure and wasteform releases are either exponentially decaying in time, in which case, the amount released can be easily determined, or release is instantaneous due to surface rinse. The default value for KPR(I) is one since calculations are only performed at requested times.

```
Enter choice: 1

This routine allows you to specify the time steps
at which output will occur.
OUTPUT file print-out control variables:

The following time intervals have non-zero print
flags, (PF).  Output will occur at these time steps
All blanks imply no output.

 T-STEP  PF  T-STEP  PF  T-STEP  PF  T-STEP  PF  T-STEP  PF  T-STEP  PF

 0) Keep these values
 1) Change values individually
 2) Change a sequence of values
Enter choice: 2

Print Flags

 0 = Print nothing (default FD)
 1 = Print concentration
 2 = Print above (1) plus material flux (default MCMC).
 3 = Print above (2) plus container breach, and waste
     form release information (FD only).

This routine will set N time step print flags to a
specified value using the following expression.

  KPR(I+J*NADD) = PRINT FLAG

where I is the number of the first time step in the
sequence, NADD is the number of time steps to be
skipped between printouts, and J is the number of
steps in the sequence (J runs from 0 to N-1)

Enter the number of the first time step in this series
Enter choice: 5

Enter the number of time steps between output, NADD
(MIN = 1, MAX = 95)
Enter choice: 10

Enter the number of times requesting output, N
(MIN = 1, MAX = 10)
Enter choice: 10

Enter the value for the print flag (0 - 3)
Enter choice: 3

OUTPUT file print-out control variables:

 The following time intervals have non-zero print
```

```
flags, (PF).  Output will occur at these time steps
All blanks implies no output.

T-STEP  PF  T-STEP  PF  T-STEP  PF  T-STEP  PF  T-STEP  PF  T-STEP  PF
  5      3   15      3   25      3   35      3   45      3   55      3
 65      3   75      3   85      3   95      3

 0) Keep these values
 1) Change values individually
 2) Change a sequence of values

Enter choice: 0
```

In the preceding example, the FD model has been specified and initial values for KPR are zero. The user selects to obtain the full printout, KPR = 3, starting at time step 5 and for every 10-th time step after this. Instructions on how to input this information are provided while running the code as shown. After specification is complete, the code returns to the output specifications menu.

If option 1, change values individually, were selected the code asks for the number of values that are to be changed and then uses this number to repeat a sequence of questions asking for the time step and print flag to be specified. Again, instructions are provided during operation of DUSTIN.

6.4.2 Number of Concentration Traces

Requesting a concentration trace requires the DUST computer code to write a file containing concentrations at a specified location as a function of time. Up to twenty locations can be specified. The output file created by DUST is called TRACECND.DAT. This file can be used directly by the graphics program GRAFXT.EXE and a plot of concentration versus time can be viewed immediately after running the DUST code.

In the MCMC model the number of concentration and flux traces as well as their locations must be identical. The reason for this is calculations are performed only at the trace locations. The DUST code performs a check to force identical flux and concentration trace locations when the MCMC model is used.

6.4.3 Location of Concentration Traces

The location of the concentration traces are determined by specifying the node (or mixing cell) at which a trace should be made. In DUSTIN the user is given the option of redefining a single trace node, or all of the trace nodes. In the following example, trace nodes had been previously specified and the user decided to change the last trace node from 50 to 60. After this, the code would print out the new values for trace nodes and ask if any further changes were desired.

```
Locations of concentration traces specified by NODE #:
```

```
(Also the location of flux traces when the mixing bath
model is used.)
Concentration trace          1 at node =          10
Concentration trace          2 at node =          20
Concentration trace          3 at node =          30
Concentration trace          4 at node =          40
Concentration trace          5 at node =          50
 0 = Keep these values
 1 = Change one
 2 = Change all individually
Enter choice: 1

Specify no. of trace (Min = 1, Max = 5)
Enter choice: 5

Enter Node for concentration trace 5
(Min = 1, Max = 100)
Enter choice: 60
```

6.4.4 Number of Flux Traces

Requesting a flux trace requires DUST to create a file containing the instantaneous mass flux, total mass (flux integrated over time multiplied by the surface area of the facility (Menu 5.2)) that has passed through that point, and mass release rate (flux multiplied by the surface area). The total mass is calculated numerically by summing the product of the flux, facility area, and time step. This estimate may be subject to large errors in the MCMC method if the time between computations is large.

If the MCMC model is specified, DUSTIN does not allow the user to input this variable and refers the user to the concentration trace section. The number of flux traces is automatically set equal to the number of concentration traces.

6.4.5 Location of Flux Traces

The location of flux traces are determined by specifying the node (or mixing cell) at which a trace is requested. If the MCMC model is used, DUST requires that the locations of the flux and concentration traces be identical. Therefore, DUSTIN refers the user to the section on specifying concentration trace locations (Menu 4.3). The input procedure for specifying location for flux traces is identical to that of concentration traces.

6.4.6 Number of Time Steps between Traces

This value specifies how frequently the trace files are updated. If the default value of 1 is used, traces are written at every time step. If a value of N is used, traces are written every N-th time step.

6.5 Facility Dimensions and Coordinates

```
                Facility dimensions and coordinates

1)  Average HEIGHT of facility (MCMC model) ..... 0.00000E+00
2)  Horizontal surface AREA of facility ......... 0.00000E+00
3)  Node coordinates (FD model)
4)  Exit to MAIN MENU
```

6.5.1 Height of the Facility

The MCMC model requires the total height of the facility. The size of each mixing cell is the total height divided by the number of mixing cells. The height must be input in centimeters.

The FD model calculates the facility height directly from the nodal coordinate input and this input is not required.

6.5.2 Surface Area

The surface area is a normalization factor that permits scaling of the concentrations (mass per unit volume) to account for the 3-D facility in a 1-D model. The volume of a compu-tational cell is the height of the cell multiplied by the surface area. Obtaining the correct concentration is important as the dose to man scales linearly with concentration. The area must be input in units of square centimeters.

6.5.3 Node Coordinates (FD model)

The FD model permits non-uniform mesh spacing. This is useful when modeling different regions which exhibit different transport characteristics. The values for the node coordinates represent depth and can be positive or negative. However, Node 1 is always the highest node (least deep) and the last node is the lowest node (greatest depth). When entering coordinate values, the coordinates must increase with depth and the user must input the coordinates in order, beginning with Node 1. (The DUSTIN code forces the user to begin with Node 1 and continue sequentially to the last node.) The distance must be in units of cm. For regularly spaced nodes, automatic generation of the nodes can be specified through the formula in the following example.

Upon entering this menu, the following description of the input requirements is presented.

```
Node coordinates
     The values for the node coordinates represent DEPTH,
and can be positive or negative.  Node 1 is always
highest (least deep), and the last node is always
lowest (greatest depth).
We recommend assigning node 1 a depth of 0.0 cm.  In
any case, coordinates must INCREASE with increasing
node number.


Press Enter to Continue.

Input of the nodal coordinates is accomplished by
using a series of cards that will automatically
calculate the coordinates using a regular sequence

In particular, this routine will ask for:
   a) the location of the first node in the sequence,  (X(I));
   b) the distance between nodes in this sequence, DELTAX, and;
   c) the fractional change in node size, XFRACT.
   d) the number of nodes in a sequence (N);

The location of each node is calculated from:
   X(I+J) = X(I) + DELTAX*(1+XFRACT)**J

  where J=0 to N-1,
```

The example below defines nodes 1 - 50 having a mesh spacing of 10 cm beginning with node 1 at x = 0.

```
   Coordinate of node 1 (cm): 0.0

Distance between each node for the nodes in this
first sequence (cm): 10.0

Fractional change of the distance between nodes over
the preceding distance: 0.0

No. of nodes that will be assigned coordinates in
this first sequence, including node 1
 (MIN = 1,  MAX = NNP = 100)
Enter choice: 50

 0 = Re-enter this sequence
 1 = Continue
Enter choice: 1
```

The DUSTIN code permits the user to re-enter the sequence if an error occurred. If the sequence is correct, the code automatically checks to make sure that every node receives a coordinate value. In this case, more nodes need to be defined and the code calculates the value of the last node and the number of nodes remaining to be defined, and asks for more input. In this example, nodes 51 - 100 have a mesh spacing of 20 cm beginning with X(51) = 500 cm.

```
No, of nodes that will be given coordinates in this
sequence. ( MIN = 1, MAX = 50)
Enter choice:  50

Coordinate of first node in sequence              2:
Cannot be less than coordinate of last node of the
previous sequence, which equals     490.000000000000      cm:
Enter value GREATER than XMIN =     490.000000000000      : 500

Increment of coordinate for each node in this
sequence, in centimeters: 20

Fractional increase (or decrease) of the increment
over its preceding increment: 0

 0 = Re-enter this sequence
 1 = Continue
Enter choice: 1
```

After completion of the input, the code prints the values requested in the form used by the DUST code.

```
Coordinate data entry complete.
The sequence of cards generated is:
     First    Number     Location    Delta X     Fract.
      Node    in Seq.                            Change
        1          50   0.00E+00   1.00E+01   0.00E+00
       51          50   5.00E+02   2.00E+01   0.00E+00
```

6.6 Initial and Boundary Conditions

The MCMC model assumes that the concentration entering the top of the modeled region is zero and because of the uni-directionality of flow, does not require a bottom boundary condition. Therefore, only the initial conditions are required. If the initial condition is zero concentration everywhere, this is the default and the code will automatically generate this when requested. If there are non-zero initial concentrations, the user specifies these through three input parameters, the number of locations to be given a value, the value, and the amount to add to that value when incrementing the location counter by 1. This procedure will be explained in detail under the FD model initial conditions section.

The following is a typical example of the Boundary and Initial Conditions session, if the transport flag indicates that the MCMC model is to be used.

```
Mixing bath model does not require boundary conditions
However, it does require initial conditions

Press Enter to Continue.


Initial condition: CONCENTRATIONS

 0 = Use DEFAULT of 0.0 initial concentration at all
     locations.
 1 = Set your own initial concentrations

Enter choice: 0
```

If the FD transport model is being used, the following menu appears.

```
                Initial and boundary conditions

1)  Initial concentrations
2)  Top boundary condition flag.....                    1
3)  Bottom boundary condition flag.....                 1
      (1 = Concentration specified  )
      (2 = Total flux specified     )
      (3 = Advective flux specified )
      (4 = Dispersive flux specified)
4)  No. of boundary condition data points.....          2
5)  Start times and values of top b.c.
6)  Start times and values of bottom b.c.
7)  Exit to MAIN MENU
```

```
Enter choice:
```

6.6.1 Initial Conditions

The initial concentration at every finite difference point must be specified. If a number of concentrations are equal or change in a regular manner, the input can be greatly simplified by entering a sequence of three numbers which represent the number of nodes (locations) at which the concentration is to be defined, the value for the concentration at the first of these nodes, and the amount to add to each successive node. DUSTIN requires that the initial conditions be specified beginning with Node 1 continuing sequentially to the last nodal point. Upon completion of specifying all concentrations, the sequence of values are printed and control is returned to the Boundary and Initial Conditions submenu. If the initial condition is zero everywhere, the user can request the code to generate the appropriate input automatically.

The instructions printed by DUSTIN when entering this menu are:

```
Initial condition: CONCENTRATIONS

 0 = Use DEFAULT of 0.0 initial concentration at all
     locations.
 1 = Set your own initial concentrations

 Enter choice: 1

This routine requires the user to define the initial
concentration at all 100 nodal points.
This is accomplished using a system that allows multiple
assignments using a sequence of 3 values.
1)  The number of nodes to be assigned a value
2)  The concentration at the first node in the sequence.
3)  The amount to add to the concentration at each node
    in the sequence.  This is usually 0.0

For example, for a system with 20 nodes. To define the
first 10 nodes the values 1 - 10 and the next 10 a
value of 0.0.  The following two sequences would be
entered.
Sequence 1 - Value 1) = 10: Value 2 = 1.0: Value 3 = 1.0
Sequence 2 - Value 1) = 10: Value 2 = 0.0: Value 3 = 0.0
```

An example in which 100 nodal points have been requested follows. The first 50 nodes have an initial concentration of one. The units of concentration are either gms/cm^3 or Ci/cm^3 depending on whether the mass inventory is input in units of grams or curies (Menu 1.3 Mass Flag).

```
This series assigns the initial concentration
beginning at Node 1
No. of nodes, including 1st, in sequence 1
 (MIN = 1, MAX = 100)
Enter choice: 50

Concentration at node 1 for 1st sequence: 1.0

Increment of initial concentration over the 50 nodes: 0.0


 0 = Re-enter this sequence
 1 = Continue
Enter choice: 1
```

At this point, the code recognizes that not all 100 nodes have been given an initial concentration and more data is requested.

```
This series starts from Node 51
No. of nodes including 1st, in sequence 2:
   (MIN = 1, MAX = 50)
Enter choice: 50

Concentration in the first node of this sequence: 0.0

Increment of initial conc. over the 50 nodes: 0

 0 = Re-enter this sequence
 1 = Continue
Enter choice: 1
```

At this point, all nodal points have a specified initial condition and the code prints out the input values in the form required by the DUST code.

```
Initial concentration data entry complete.

The sequence of cards generated is :
First Node    Number     Concentration    Change in
in Seq.       in Seq.                     Concentration
     1          50        1.00E+00          0.00E+00
    51          50        0.00E+00          0.00E+00
```

6.6.2 Top Boundary Condition Flag

Four choices for boundary conditions are allowed within the DUST code. The concentration, total flux, advective flux, or diffusive/dispersive flux can all be specified as a function of time. These are described in detail in Section 2.6.

This input value selects the boundary condition from among these choices. The default value requires the concentration to be specified.

6.6.3 Bottom Boundary Condition Flag

The choices are identical to those at the top boundary as described in 6.6.2.

6.6.4 Number of Boundary Condition Data Points

All boundary conditions are specified as a function of time through a table containing the value of the boundary condition and the time in years. At any given simulation time, the value of the boundary condition is determined through interpolation of this table. The last time in the boundary condition table should be greater than or equal to the maximum simulation time. If this is not done, unpredictable results may occur. The minimum number of data points required to specify the interpolation table is 2. The maximum number allowed by the code is 10.

6.6.5 Boundary Condition Table for the Top Boundary

Boundary conditions (BC) are input as ordered pairs of time (years) and BC value (where the units are consistent with previous input, e.g., if mass is input in curies, mass units for the BC are in curies).

The following example has 4 data points in the table (specified in Menu 6.4), a maximum simulation time of 100 years (specified in Menu 2.7) and sets the concentration to 1.0 between 0 and 10 years and 0.0 after 10.01 years. Between 10 and 10.01 years the concentration varies linearly between 1 and 0. Upon entering this submenu, the code prints out the existing values for the BC (all zero by default in the example). After a decision has been made to change the values, the code prompts the user for the first concentration value and forces the first time in the table to 0.0 years.

After this, the code prompts the user for the time and boundary value. These are input on a single line separated by a space. After all of the boundary points are specified, the table is printed for review by the user.

```
    Current Values:
Time (yrs)      Boundary Value
  0.00E+00            0.00E+00
  0.00E+00            0.00E+00
  0.00E+00            0.00E+00
  0.00E+00            0.00E+00

Do you wish to change these values. (0 = No, 1 = Yes)
Enter choice: 1

Value of boundary condition at TIME = 0.0
Enter concentration: 1.0

For ordered pair # 2
Enter time (in yrs) and corresponding value of B.C.
10 1.0

For ordered pair # 3
Enter time (in yrs) and corresponding value of B.C.
10.01 0.0

For ordered pair # 4
Enter time (in yrs) and corresponding value of B.C.
100 0.0


Time and boundary value entries complete.

Time (yrs)      Boundary Value
  0.00E+00            1.00E+00
  1.00E+01            1.00E+00
  1.00E+01            0.00E+00
  1.00E+02            0.00E+00

Press Enter to Continue.
```

6.6.6 Boundary Condition Table for the Bottom Boundary

This procedure is identical to that of the top boundary. For details see Section 6.6.5.

6.7 Water Flow and Moisture Content

For the MCMC model, the user is permitted to input a single value for the Darcy velocity and the moisture content. The FD model permits the Darcy velocity to be obtained as a function of time through tabular input in an approach similar to that of specifying the boundary conditions. The moisture content is permitted to vary spatially. The values for the Darcy velocity and moisture content should be obtained from numerical simulations with site specific data. The menu is:

```
        Water flow and moisture content


1)  Darcy Velocity
2)  Moisture content values and location
3)  Exit to MAIN MENU
```

6.7.1 Darcy Velocity

For the MCMC model, the DUSTIN code prints the current value for the Darcy velocity, asks if a change is needed, and if so, asks for the value of the Darcy velocity (cm/s).

For the FD model, a table of velocity versus time may be input or a single value for the Darcy velocity may be used. If a single value is used, the code asks the user for that value and creates the input table by specifying this value at t = 0 and t = TMAX (Menu 2.7). If a table is input, the velocity at any simulation time is calculated through linear interpolation using the table. If the last time value in the table is less than the maximum simulation time, unpredictable results may occur.

In the following example, the user has decided to specify an increase in velocity over time between 0 and 1000 years. DUSTIN prints current values for the table (0 by default) and asks if a change is requested.

```
Finite-difference model permits a table of Darcy
velocity versus time

Current values for Darcy Velocity vs. Time
Time (yrs)    Darcy Velocity (cm/s)
  0.00E+00                0.00E+00
  0.00E+00                0.00E+00

Do you wish to change these values. (0 = No, 1 = Yes)
Enter choice: 1
```

At this point, the user is provided a choice of using a single value or inputting a table of values. If a table of values is desired, the user inputs the number of points in the table and the code then prompts the user for the values. The code forces the first time value to be at zero years.

```
 1) Enter a single value for Darcy Velocity
 2) Enter a table of Darcy Velocity versus time
 3) Exit
Enter choice: 2


No. of (time, Darcy velocity) pairs
 (MIN = 2, MAX = 10)
Enter choice: 2

Darcy velocity at TIME = 0.0, in cm/sec: 3.5e-7

Enter time T and VDAR(T), in yrs and cm/sec

TIME (yrs): 1000

Darcy velocity (cm/sec): 7.0e-7

Time and Darcy velocity data entries complete.

Time (yrs)    Darcy Velocity (cm/s)
  0.00E+00                3.50E-07
  1.00E+03                7.00E-07
```

6.7.2 Moisture Content Values

For the MCMC model, the DUSTIN code prints the current value for the moisture content, asks if a change is needed, and if so, asks for the value of the moisture content. The code permits the moisture content, volume of water per volume of the system, to range between 0.0 and 1.0. Typically values fall within a more narrow range, i.e., from 0.05 in very arid sites to 0.5 in saturated sites.

For the FD model, the moisture content may vary with position. The values for moisture content should be determined from detailed simulations of the flow around the facility. In assigning moisture content values, the user must specify a value for every control volume. If the moisture content values remain constant or change linearly between control volumes for a region of the modeled domain, automatic generation of the moisture content can be prescribed.

The DUSTIN code forces the user to enter the moisture content for each control volume (node), beginning with Node 1 and continuing sequentially until all nodes are specified. When

entering this menu, existing values are printed in the form required as input by DUST and the user is asked if a change is desired.

```
Moisture content values and location

The current sequence of cards generated is :

First Node    Number      Moisture      Change in
in Seq.       in Seq.     Content       Moisture Cont
         0            0    0.00E+00           0.00E+00

Do you wish to change these values (0 = No, 1 = Yes)
Enter choice: 1

 0 = Moisture content is equal at all nodes
 1 = Moisture content varies at different nodes
Enter choice: 1
```

If the moisture content is constant (0 entered on the previous menu), the code asks for the value. If the moisture content changes with location, the following instructions are printed.

```
This routine requires the user to define the initial
moisture content at all 100 nodal points.
This is accomplished using a system that allows multiple
assignments using a sequence of 3 values.
1)  The number of nodes to be assigned a value
2)  The moisture content at the first node in the sequence.
3)  The amount to add to the moisture content at each
    node in the sequence.  This is usually 0.0
```

In the following example, the number of nodes has been specified to be 100 and the moisture content is set to 0.25 for the first 50 nodes and 0.3 for the last 50 nodes.

```
The first node in this sequence is node 1
```

```
No. of nodes in 1st sequence
 (MIN = 1, MAX = 100)
Enter choice: 50

Moisture content at node 1 of 1st sequence:  (Min = 0.0, Max = 1.0) : 0.25

Increase or decrease in moisture content over
each of the 50 nodes: 0.0

 0 = Re-enter this sequence
 1 = Continue
Enter choice: 1
```

At this point, the code recognizes that only 50 of the 100 nodes have been given a value for moisture content. Therefore, it prints the instructions out and requests more input. Notice that the code begins this sequence at Node 51, the first undefined node.

```
This routine requires the user to define the initial
moisture content at all 100 nodal points.
This is accomplished using a system that allows multiple
assignments using a sequence of 3 values.
1)  The number of nodes to be assigned a value
2)  The moisture content at the first node in the sequence.
3)  The amount to add to the moisture content at each
    node in the sequence.  This is usually 0.0

The first node in this sequence is node 51
No. of nodes including 1st in sequence 2:
 (MIN = 1, MAX = 50)
Enter choice: 50

Moisture content at node 1 of this sequence:  (Min = 0.0, Max = 1.0) : 0.3

Increase or decrease in moisture content over
each of the 50 nodes: 0.0


 0 = Re-enter this sequence
 1 = Continue
Enter choice: 1
```

Upon specifying all moisture content values the code prints out the input cards needed by the DUST code.

```
Moisture content data entry complete.

The sequence of cards generated is :

First Node    Number      Moisture      Change in
in Seq.       in Seq.     Content       Moisture Cont
       1          50     2.50E-01           0.00E+00
      51          50     3.00E-01           0.00E+00
```

6.8 Container Parameters

The DUST computer program allows up to 300 different containers each with a unique time to failure. The MCMC model does not allow localized failure to occur. Therefore, it requires only the number of containers, the time to failure and location of each container. The FD model permits up to 20 different localized container failure rates to be applied to the containers. Therefore, it requires input on the rate parameters, and integer flags that specify which set of rate parameters should be used for each container. The container menu is:

```
                    Container parameters

1)  No. of containers ..................................... 0
2)  Time of general failure for each container
3)  Location of each container
Items 4 - 7 are required only by the FD model
4)  No. of failure types for local failure ............... 0
5)  Corrosion model flag for each container type
6)  Loc. failure parameters for each cont. type
7)  Loc. failure parameter assignments to containers
8)  Exit to MAIN MENU
```

6.8.1 Number of Containers

This input variable provides the total number of mixing cells or control volumes that have a wasteform source.

6.8.2 Time of General Failure

Each container has a time of general failure after which the container no longer provides a barrier to release from the wasteform. These times should be estimated based on the material,

thickness, and expected degradation rates. Information is available on corrosion rates for carbon and stainless steels in soil systems [Romanoff, 1957; Gerhold, 1981; Sullivan, 1989].

The failure time must be input for each container in units of years. Upon entering this submenu, the code prints the current values for failure times and allows the user to change each one of these times independently or set a series to a single value.

```
Time of general failure of each container

Con-    Time of       Con-    Time of       Con-    Time of       Con-    Time of
tainer  failure(yrs)  tainer  failure(yrs)  tainer  failure(yrs)  tainer  failure(yrs)
   1    0.00E+00        2     0.00E+00        3     0.00E+00        4     0.00E+00
   5    0.00E+00        6     0.00E+00        7     0.00E+00        8     0.00E+00
   9    0.00E+00       10     0.00E+00       11     0.00E+00       12     0.00E+00
  13    0.00E+00       14     0.00E+00       15     0.00E+00       16     0.00E+00
  17    0.00E+00       18     0.00E+00       19     0.00E+00       20     0.00E+00

 0 = Keep these times
 1 = Change one
 2 = Change all individually
 3 = Change a series to one value
Enter choice: 3
```

In changing a single value, the code asks for the node number and the failure time. When changing a series to one value, the following instructions are provided on the screen when running DUSTIN. In the example, the user has previously specified that there are 20 containers and then sets the failure time of the first 10 containers at 10 years and the last 10 containers at 20 years. This is achieved through input of three values: a) the value for the first container in this sequence; b) the total number of containers in the sequence; and c) the failure time. After a sequence has been completed, the current failure times are printed and the user is asked if more changes are required.

```
This sequence will assign containers I through I+N the
same value for the time of breach


Enter the number of the first container in this
sequence (MIN = 1, MAX = 20):
Enter choice: 1

Number of containers to be assigned a value
(MIN = 1, MAX = 20):
Enter choice: 10
```

```
Enter the value for the time of breach (yrs) in this sequence.    10
```

The process was continued for the remaining containers. Output of the current values for failure times follows:

```
Enter the number of the first container in this
sequence (MIN = 1, MAX = 20):
Enter choice: 11

Number of containers to be assigned a value
(MIN = 1, MAX = 10):
Enter choice: 10

Enter the value for the time of breach (yrs) in this sequence.    20

Con-    Time of      Con-    Time of      Con-    Time of      Con-    Time of
tainer  failure(yrs) tainer  failure(yrs) tainer  failure(yrs) tainer  failure(yrs)
   1    1.00E+01        2    1.00E+01        3    1.00E+01        4    1.00E+01
   5    1.00E+01        6    1.00E+01        7    1.00E+01        8    1.00E+01
   9    1.00E+01       10    1.00E+01       11    2.00E+01       12    2.00E+01
  13    2.00E+01       14    2.00E+01       15    2.00E+01       16    2.00E+01
  17    2.00E+01       18    2.00E+01       19    2.00E+01       20    2.00E+01

 0 = Keep these times
 1 = Change one
 2 = Change all individually
 3 = Change a series to one value
```

6.8.3 Location of the Containers

Each container must be assigned to a unique location. This is accomplished by DUSTIN in a similar fashion as specifying the failure times. The user is permitted to change each value independently, or change a sequence of values. If a sequence of values are to be created, four values are needed: a) the number of the first container in the sequence; b) the location (cell number) of the first member of the sequence; c) the distance between (number of cells) adjacent containers; and d) the number of values to be assigned in the sequence. The default value for container location is zero. Failure to define this number will cause the DUST code to fail.

The equation used to generate this sequence is presented in the menu as shown below. In the example problem, the user has specified that the first container is in node 20 and the remaining containers are in the 19 adjacent cells. The DUSTIN code requires that each container location be

defined. If the user has not defined all locations the code returns to the location specification menu and requires further input.

```
This will assign containers I through I+N the
value for the node number using the following
expression.
 NELCON(I+JN) = NUM0 + JN*NADD
 where JN ranges from 0 to N

Enter the number of the first container in this
sequence, I; (MIN = 1, MAX = 20):
Enter choice: 1

Enter the node number of the first container in this sequence, NUM0.
Enter choice: 20

Enter the number of nodes between containers, NADD
(MIN = 1, MAX = 80):
Enter choice: 1

Number of containers to be assigned a value, JN
(MIN = 1, MAX = 20):
Enter choice: 20
```

Upon completion of the input, the values are translated into cell (node) numbers and the results are printed for review.

Container	Node	Container	Node	Container	Node	Container	Node
1	20	2	21	3	22	4	23
5	24	6	25	7	26	8	27
9	28	10	29	11	30	12	31
13	32	14	33	15	34	16	35
17	36	18	37	19	38	20	39

```
0 = Keep these locations, return to menu
1 = Change one location
2 = Change all locations individually
3 = Change a sequence of locations
```

6.8.4 Number of Failure Types (FD)

The FD model permits localized failure. The data in the model has been specialized to pitting corrosion but it may be generalized to provide an early localized failure for any process. Up to 20 different localized failure rates may be specified. If localized failure is not desired leave this value equal to the default value, 0.

6.8.5 Corrosion Model Flag

All containers must have a specified time to failure. However, each container type may also fail due to local corrosion. The choice is specified through setting this flag to 1 for local corrosion. This is used only if the number of failure types is non-zero. The structure of the input routine for this value is identical to that for specifying the time to failure and will not be repeated. This is useful when the user desires to model a portion of the containers failing by local corrosion and the remainder by a general failure time. The code user could specify more than one container type and require that one container type does not undergo local corrosion by setting this flag to zero.

6.8.6 Localized Failure Parameters

The model for localized failure has been presented in Section 2.4.2. The model requires six parameters (the number of penetrating pits per container, the area of the container, the area scaling factor, the container thickness, and the two empirically determined rate parameters used to describe pit growth). Suggested values for these parameters are presented in Appendix C. The DUSTIN code permits the user to change every single variable independently through the use of the submenus. Upon entering this submenu, the following instructions are printed.

```
The localized failure model has the form:
 area breached = npits*pi*(h**2-d**2)
 npits = number of pits per container.
 d = the container thickness.
 h = depth of the local penetration
 h = Kt**N * (A/372)**a
 K,N,and a = empirically determined rate parameters
 A = area of the waste form and t is the time (yrs)
 This model was developed for pitting of carbon
 steels.  Application to other materials or failure
 modes should be done with caution
```

The current values for these parameters are then printed and the user is asked if a change is requested.

```
Thick      N          K          Area       A-scale    No. of Pen.    Index

0.00E+00   0.00E+00   0.00E+00   0.00E+00   0.00E+00   0.00E+00           1
0.00E+00   0.00E+00   0.00E+00   0.00E+00   0.00E+00   0.00E+00           2

Do you wish to change any of these parameters (0 = No, 1= Yes)
Enter choice: 1
```

The code then prints out the container types that require localized corrosion parameters and asks which container type will receive changes.

```
The following container types require localized
failure parameters:
Index = 1
Index = 2

Enter container type index (MIN = 1, MAX = 2)
Enter choice: 2
```

Here container 2 receives the changes. The code then prints out information on the input variables in the failure parameter menu. A full discussion of these variables can be found in [Sullivan, 1989].

```
The following are the range and recommended values
for 55 gallon carbon steel drums.  If other materials
or containers are used, check your input carefully.

0) Exit
1) Thickness (cm):                                    0.127 - 0.152
   For HIC's thicknesses are generally                0.9 - 1.0
2) Pitting parameter N:                               0.0 - 0.92
                                  Mean value -        0.39
3) Pitting parameter K (cm/yr**N)):                   0.03 - 0.15
                                  Mean value -        0.0737
4) Surface area (55 gallon drum) (cm**2):             2.1E4
5) AREA SCALING PARAMETER, a:                         0.08 - 0.32
                                  Mean value -        0.15
6) Number of penetrations per container:              500 -  5000
   For carbon steels, studies indicate a
```

```
   mean value of 0.05 pits/cm**2.  For a
   55 gallon drum (Area = 2.1E4 cm**2)
   This implies a mean value of:              1000
7) Input all values

Input selection
Enter choice: 7
```

In this case, all parameters will be changed. The code then prints the following and requests the input for all parameters on one line separated by spaces.

```
CONTAINER TYPE 2

Input the following localized failure parameters
on the following line for Container type 2
Thickness     N      K      AREA      A-SCALE      No. Penetrations
 0.15         0.4    0.08   2.1e4     0.15         1001
```

If the change was to be made only to a single parameter, the code prints the parameter name and asks for the input value. It then returns to the parameter menu and asks if another parameter is to be changed. In the example, the code asks if the user wants to continue data entry. If further input is requested, the code asks which material is to receive changes. If input of local failure parameters is complete, control is returned to the container parameter menu (i.e., the menu containing information on number of containers, time of failure, etc.). Upon returning to that menu, the values for the rate parameters are printed.

```
Thick       N           K           Area        A-scale     No. of Pen.     Index

1.50E-01  3.90E-01  1.00E-01  2.10E+04  1.50E-01  1.00E+03          1
1.50E-01  4.00E-01  8.00E-02  2.10E+04  1.50E-01  1.00E+03          2
```

6.8.7 Assignment of Localized Failure Parameters to Each Container

If more than one set of container types is requested in Menu 8.4, the user must specify the container type for each container. This assigns local container failure parameters to each container. The procedure is similar to that used in specifying times to failure, the user can change any single

container type or a sequence of container types. Upon entering this menu, the code prints out the existing values and requires reassignment to non-zero values.

```
                Container types are assigned to all containers

Container   Node#   Container type    Container   Node#   Container type
        1     20                0            2     21                0
        3     22                0            4     23                0
        5     24                0            6     25                0
        7     26                0            8     27                0
        9     28                0           10     29                0
       11     30                0           12     31                0
       13     32                0           14     33                0
       15     34                0           16     35                0
       17     36                0           18     37                0
       19     38                0           20     39                0

Container types have not been assigned
Enter assignment

  1 = Change one type assignment
  2 = Change all assignments individually
  3 = Change a series to one value
Enter choice: 3
```

To reassign a series of container types three input variables must be supplied, the container number of the first container in the series, the number of containers in the series, and the container type for the series. In this example, containers 1 - 10 are given type 1 failure parameters and containers 11 - 20 are specified as type 2 containers.

```
This will assign containers I through I+N the
same value for container type.

Enter the number of the first container in this
sequence (MIN = 1, MAX = 20)
Enter choice: 1

Number of containers to be assigned a value
(MIN = 1, MAX = 20)
Enter choice: 10

Enter the value for the container type.
(Min = 1 and MAX = 2)
```

```
Enter choice: 1
```

At this point, only 10 of the 20 containers have been reassigned. The DUSTIN code automatically asks for a continuation until all 20 containers are assigned a non-zero value.

```
Container types have not been assigned
Enter assignment

 1 = Change one type assignment
 2 = Change all assignments individually
 3 = Change a series to one value
Enter choice: 3

This will assign containers I through I+N the
same value for container type.

Enter the number of the first container in this
sequence (MIN = 1, MAX = 20)
Enter choice: 11

Number of containers to be assigned a value
(MIN = 1, MAX = 10)
Enter choice: 10

Enter the value for the container type.
(Min = 1 and MAX = 2)
Enter choice: 2
(MIN = 1, MAX = 10)
Enter choice: 10

Enter the value for the container type.
(Min = 1 and MAX = 2)
Enter choice: 2
```

After the container assignments are complete, the values are printed for review.

Container	Node#	Container type	Container	Node#	Container type
1	20	1	2	21	1
3	22	1	4	23	1
5	24	1	6	25	1
7	26	1	8	27	1
9	28	1	10	29	1
11	30	2	12	31	2

```
      13      32              2          14      33              2
      15      34              2          16      35              2
      17      36              2          18      37              2
      19      38              2          20      39              2

 0 = Keep these assignments; go to menu
 1 = Change one type assignment
 2 = Change all assignments individually
 3 = Change a series to one value
Enter choice: 0
```

6.9 Wasteform Parameters

The DUST computer code simulates a wasteform in every control volume (or mixing cell) that has a container (the maximum number of containers is 300). Each wasteform is permitted to have a unique inventory. However, the code permits only twenty different wasteform types to be modeled. Each wasteform type is represented by a unique set of release rate parameters.

Again, the choice of the transport model has a large impact on the amount and type of input required. The MCMC model allows an exponentially decaying release rate or a rinse release. The FD model allows these two release mechanisms plus a diffusion release mechanism. Diffusive releases are dependent on the geometry and dimensions of the wasteform. This requires additional input. Either rectangular or cylindrical geometry can be modeled. The models have been presented in detail in Section 2.5 and will not be repeated.

The wasteform parameters menu is:

```
                    Wasteform parameters

1)  No. of waste types ..................................... 0
2)  Finite difference model release rate parameters
3)  Mixing bath model release rate parameters
4)  Initial amount of XXXXXXX in each container
5)  Waste type assignment to each container
6)  Exit to MAIN MENU

Enter choice:
```

6.9.1 Number of Waste Types

The number of waste types is the number of wasteforms having unique release rate parameters. The maximum value permitted in DUST is 20.

6.9.2 Finite Difference Model Release Rate Parameters

Upon requesting to alter the finite difference release rate parameters, the following menu is printed.

```
Finite difference model release rate parameters:
 0 = Exit
 1 = Specify geometry of the wasteform
 2 = Specify release rate, dimensional, and inventory fraction parameters
Enter choice: 1
```

For diffusion controlled release the code contains analytical solutions for release from cylindrical or rectangular wasteforms [Section 2.5.3]. Therefore, the geometry must be specified. The default choice is cylindrical geometry. If diffusional release from a rectangular wasteform is modeled, the geometry flags need to be redefined.

If the geometry is to be redefined, the code prints out existing values for the flags, defines the flags, and asks if a change is desired.

```
Waste type   Geom Flag    Waste Type   Geom Flag
        1           0             2           0

Enter flags for wasteform geometry

 0 = Cylindrical wasteform
 1 = Rectangular wasteform


 0 = Keep these values, return to menu
 1 = Change one
 2 = Change all individually
 3 = Change a series to one value
Enter choice: 2
```

In this example, the user has decided to change each flag individually. The code then prompts the user for the flag values.

```
Geometry flag of waste type 1
Enter choice: 1

Geometry flag of waste type 2
Enter choice: 0

Geometry flag entries complete.
```

At this point, the code prints the values for the flags and provides the user with an opportunity to make further changes or return to the menu which accesses the release rate parameter menu below. At this time, the example below indicates that release rate parameters require definition.

```
Finite difference model release rate parameters:
 0 = Exit
 1 = Specify geometry of the wasteform
 2 = Specify release rate, dimensional, and inventory fraction parameters
Enter choice: 2
```

The release rate parameter menu follows. Again, the user can change all parameters independently through the menu. Upon entering this menu, the current values are printed and the user is asked if changes are desired for one or all waste types. In this example, two waste types (Menu 9.1) have been requested and the FD transport model is specified.

```
The finite difference model requires release rate,
inventory fraction available for each release mechanism,
and parameters that define the size of the wasteform.
You can enter parameters for a single waste type or for all waste types

Current values for the parameters are:
Wasteform                      1          2
Rinse Fraction           :   0.00E+00   0.00E+00
Diffusion fraction       :   0.00E+00   0.00E+00
Dissolution fraction     :   1.00E+00   1.00E+00
Partition coefficient    :   0.00E+00   0.00E+00
Diffusion coefficient    :   0.00E+00   0.00E+00
```

```
Fractional Rel Rate     :    0.00E+00   0.00E+00
Wasteform radius        :    0.00E+00   0.00E+00
Wasteform volume        :    0.00E+00   0.00E+00

Press Enter to Continue.


 0 = Return to menu
 1 = Change one set of release rate parameters
 2 = Change all release rate parameters
Enter choice: 2
```

The code will cycle through all of the different waste types asking for changes to the release parameters. In this example, waste type 1 has been defined and the code asks for changes to waste type 2.

```
WASTEFORM TYPE:  2

Release Rate parameter menu

     0 = Exit
     1 = Change all release rate parameters
     2 = Change inventory fraction available for rinse and diffusion
     3 = Fractional release rate (Bulk Dissolution)

           Item's 4) -  8) are used only by the
           finite difference model
     4 = Change wasteform partition coefficient
     5 = Change wasteform diffusion coefficient
     6 = Change half-width/radius of the wasteform
     7 = Change half-height of the wasteform
     8 = Change wasteform volume
Enter choice: 1
```

The first time through this menu it is necessary to define all of the parameters. For the finite difference model, there are three release mechanisms: rinse, diffusion, and uniform. Each of these is independent. The amount of mass available for release by each mechanism is the total mass in the wasteform (Menu 9.5) multiplied by the fraction of mass available for each mechanism. These are input as the fraction available for rinse and the fraction available for diffusion. The fraction available for uniform release is determined by requiring that all three sum to 1.

Item 3 on the menu, the fractional release rate, is the fraction of the uniform release fraction that is released per year. For example, if a wasteform had an initial inventory of 1 Curie and 10% of the inventory was available for uniform release, a fractional release rate of 0.05 per year would

release 0.005 Ci/yr (this value would be adjusted to account for decay) due to uniform release. Additional releases would occur due to the diffusion and rinse mechanisms. This parameter is also used by the MCMC model.

Item 4, the wasteform partition coefficient, can be used to represent control of release by reversible chemical interactions with the wasteform, for example sorption on dewatered ion exchange resins. If this value is zero, the entire rinse mass (total mass multiplied by rinse fraction) is released into solution upon breach of the container subject to solubility limits. If the partition coefficient is non-zero, releases from this wasteform can be negative. The model performs a mass balance and determines the distribution of contaminants subject to the partition coefficient. Therefore, contaminants in solution may be removed causing a negative release for this wasteform. When using the partition coefficient the code user must be extremely careful so as not to account for sorption effects twice as there is also a distribution coefficient in the transport model. This is discussed in detail in Section 2.5.2.

Item 5, wasteform diffusion coefficient, is used when the diffusive release fraction is non-zero. The code has analytical solutions for finite-sized cylindrical and rectangular wasteforms, see Section 2.5.3. Values for the diffusion coefficient depend on the waste stream and solidification agent. The Technical Position on Wasteform [Lohaus, 1991] requires that the diffusion coefficient be smaller than 10^{-6} cm^2/s for solidified wastes. A collection of diffusion coefficient values is presented in [Sullivan, 1989].

Diffusive releases depend strongly on the wasteform dimensions. For a fixed value of the diffusion coefficient, larger wasteforms will have a lower cumulative fractional release as compared to smaller ones. Therefore, it is crucial to input the proper dimensions. In many cases, in order to improve the numerical accuracy of the FD model, it may be necessary to model a single wasteform using several control volumes. In this case, the wasteform dimensions must be input as the true dimensions. To properly model the total release, the wasteform mass should be evenly divided among all control volumes representing the wasteform. For example, if 10 control volumes were used to model a cylindrical wasteform having a height of 50 cm, a radius of 25 cm and with an initial inventory of 40 curies, the proper way to model this would define 10 wasteforms all with the same release mechanisms, i.e., all the same wasteform type. The radius of this wasteform type is 25 cm and the volume is 9.82E4 cm^2. The initial inventory for each of these 10 wasteforms is 4 curies.

For rinse and uniform release, the dimensions are unimportant in estimating wasteform release. Therefore, if a wasteform is divided, the initial mass of the contaminant should be divided uniformly between the control volumes.

Item 6, is a dual purpose variable. For cylindrical wasteforms, it is the radius. For rectangular wasteforms it is the half-width. This variable is only used for predicting diffusion release. The analytical release models require the dimensions of the wasteform. In DUST, these are specified by supplying the radius and volume for cylindrical wasteforms. The half-width, half-height, and the volume combine to define the geometry of rectangular wasteforms.

Item 7, is the half-height of a rectangular wasteform. This variable is not used for cylindrical wasteforms.

Item 8, is the volume of the wasteform.

If the mass fraction available for diffusion is zero for a waste type, items 5 - 8 are not required as input.

The following example requests the properties for waste type 2 which was previously defined as having cylindrical geometry. The user has requested to change all variables. The code prompts the user for each variable and gives the required units.

```
WASTEFORM TYPE:  2
Fraction of waste's inventory available for SURFACE RINSE: 0.1
Fraction of waste's inventory available for DIFFUSION: 0.8
Fractional Release Rate (1/yr): 1e-3
Wasteform partition coefficient (cm**3/gm): 0.0
Diffusion coefficient inside wasteform (cm**2/s): 1e-9
Radius of cylindrical waste (cm): 25
Volume of wasteform (cm^3): 1.67e5
Wasteform type parameters complete.
```

Upon completing the input routine, the code prints out the current values for the release rate parameters and asks if further changes are requested.

```
Current values for the parameters are:
Wasteform                    1          2
Rinse Fraction          :    1.00E-01   1.00E-01
Diffusion fraction      :    9.00E-01   8.00E-01
Dissolution fraction    :    0.00E+00   1.00E-01
```

```
Partition coefficient :    0.00E+00  0.00E+00
Diffusion coefficient :    1.00E-09  1.00E-09
Fractional Rel Rate   :    0.00E+00  1.00E-03
Wasteform radius      :    5.00E+01  2.50E+01
Wasteform volume      :    3.00E+06  1.67E+05

Press Enter to Continue.



 0 = Return to menu
 1 = Change one set of release rate parameters
 2 = Change all release rate parameters
Enter choice:
```

6.9.3 Mixing Cell Model Release Rate Parameters

The MCMC model permits only two release mechanisms: rinse and uniform release. In this rinse model, there is no wasteform partitioning coefficient. Upon container failure, all mass is released into solution. If the soil distribution coefficient is non-zero, the mass is distributed between the soil and water instantaneously. The uniform release parameter has the same definition as in the FD model. Again, the release rate for this model decreases exponentially due to radioactive decay.

Two release rate parameters, the fraction available for rinse and the fractional release rate, completely describe the release for the MCMC model. The input routine is similar to that for the FD model. When using the Release Rate Parameter Menu shown above, the code prevents the user from defining variables that are not needed for this model.

6.9.4 Initial Inventory

The user must supply the initial inventory for each waste container. The units for inventory are specified by menu item 1.3. Input can be done for each individual container or a series of wasteforms may be assigned an identical inventory. In the following example, the user has previously requested 20 waste containers (Menu 8.1) with the inventory units of curies. The code prints the current inventory (all zero by default) and asks for changes. In this case, a series of inventories will be set to a single value.

```
Input initial inventory in each container

Initial inventory in curies in the wasteforms:

Container   Inv.     Container   Inv.     Container   Inv.     Container  Inv.
    1    0.00E+00        2    0.00E+00        3    0.00E+00        4    0.00E+00
    5    0.00E+00        6    0.00E+00        7    0.00E+00        8    0.00E+00
```

```
   9   0.00E+00      10   0.00E+00      11   0.00E+00      12   0.00E+00
  13   0.00E+00      14   0.00E+00      15   0.00E+00      16   0.00E+00
  17   0.00E+00      18   0.00E+00      19   0.00E+00      20   0.00E+00


 0 = Keep these mass values
 1 = Change one
 2 = Change all individually
 3 = Change a series to one value

Enter choice: 3
```

The next few lines define waste containers 1 - 20 as having an initial inventory of 10 Curies.

```
This will assign containers I through I+N the
same value for the initial inventory

Enter the number of the first wasteform in this
sequence (MIN = 1, MAX = 20):
Enter choice: 1

Number of wasteforms to be assigned a value
(MIN = 1, MAX = 20):
Enter choice: 20

Enter the value for the initial inv. in this sequence.  10
```

After completing the input, the current values for the inventory are printed and the user is asked if further changes are required.

```
Container   Inv.     Container   Inv.     Container   Inv.     Container  Inv.
    1   1.00E+01        2   1.00E+01        3   1.00E+01        4   1.00E+01
    5   1.00E+01        6   1.00E+01        7   1.00E+01        8   1.00E+01
    9   1.00E+01       10   1.00E+01       11   1.00E+01       12   1.00E+01
   13   1.00E+01       14   1.00E+01       15   1.00E+01       16   1.00E+01
   17   1.00E+01       18   1.00E+01       19   1.00E+01       20   1.00E+01


 0 = Keep these mass values
 1 = Change one
 2 = Change all individually
```

```
 3 = Change a series to one value

Enter choice:
```

6.9.5 Waste Type Assignment to Each Container

This variable acts as a flag that links a set of wasteform release rate parameters to a specific container and is required only if more than one set of release parameters are defined. The input routine is similar to that used for inventory assignment. The user has the option of changing a single waste type assignment, changing all waste type assignments individually, or changing a sequence of assignments to a single value.

Upon entering this menu, the code prints the current values and asks the user if further changes are required. In this example, the first 10 containers are assigned waste type 1.

```
Waste type assignment to each container
Wasteform types are assigned to all containers

Wasteform   Node#  Wasteform type   Wasteform   Node#  Wasteform type
        1     20               0           2     21               0
        3     22               0           4     23               0
        5     24               0           6     25               0
        7     26               0           8     27               0
        9     28               0          10     29               0
       11     30               0          12     31               0
       13     32               0          14     33               0
       15     34               0          16     35               0
       17     36               0          18     37               0
       19     38               0          20     39               0

 1 = Change one type assignment
 2 = Change all assignments individually
 3 = Change a series to one value
Enter choice: 3

This will assign containers I through I+N the
same value for wasteform type.

Enter the number of the first container in this
sequence (MIN = 1, MAX = 20)
Enter choice: 1

Number of wasteforms to be assigned a value
(MIN = 1, MAX = 20)
Enter choice: 10
```

```
Enter the value for the wasteform type.
(Min = 1 and MAX = 2)
Enter choice: 1
```

At this point, the program would print out the existing values for waste type assignment and require the user to input more values. The code requires that all waste type assignments are non-zero before allowing the user to return to the wasteform menu.

6.10 External Source/Sink Terms

The FD transport model permits the user to supply an external volumetric source/sink term. This term represents the rate of injection/removal of mass into the volume represented by one finite difference control volume in the system. The external source term is specified as a function of time through tabular input. Values are obtained through interpolation using the table. In the DUST code this term has units of mass/cm^3/s. The mass units are determined by the activity flag, Menu 1.3. If the mass units are curies, the DUST code internally transforms this into grams to maintain consistency. The main menu for Source/Sink parameters follows.

```
        Source/Sink parameters - FD Model Only

1)  No. of nodes with a source.....................0
2)  No. of source profiles.........................0
3)  No. of source data points......................0
4)  Times and values of sources
5)  Locations of sources
6)  Source profile assignment to nodes with source
7)  Exit to MAIN MENU
```

If there are no external sources, items 4 - 6 of the menu are not used by the DUST code. DUSTIN prevents the user from inputting values for these items when the number of source nodes is zero.

6.10.1 Number of Source Nodes

The total number of locations where a source exists ranges up to 500, however, it is not to exceed the number of nodal (control volume) points specified in Menu 1.4.

6.10.2 Number of Source Profiles

The DUST code accepts up to 8 different source profiles. This value must be non-zero if the number of source nodes is non-zero.

6.10.3 Number of Source Data Points

Each source profile table must contain at least two points and no more than 8 points. The specified number of data points applies to every profile.

6.10.4 Times and Values of the Sources

The magnitude of the source is specified in a table which contains a set of ordered pairs of time (years) and source strength (mass/cm^3/s). The code prompts the user for the ordered pairs to be entered on a single line.

In the following example, the user previously requested 2 source profiles with 4 data points. The code prints the current values for the table and then asks if further changes are requested. In this case, profile number 1 has a concentration of 1E-5 Ci/cm^3/s between 0 and 10 years. This decreases to zero at 10.01 years and remains there until 1000 years. Interpolation is used to determine the calculation at times not in the table. Therefore, the first time should be the problem start time (normally 0) and the last time should be greater than the maximum problem time, Menu 2.7.

```
Profile #      1                    2
      Time     Source       Time    Source       Time     Source

  0.00E+00  0.00E+00  0.00E+00  0.00E+00
  0.00E+00  0.00E+00  0.00E+00  0.00E+00
  0.00E+00  0.00E+00  0.00E+00  0.00E+00
  0.00E+00  0.00E+00  0.00E+00  0.00E+00

Enter tables of volumetric source strength vs. time:

  0 = Exit
  1 = Assign one table
  2 = Assign all tables
Enter choice: 2

Enter time (in yrs) and corresponding value of
volumetric source strength in units of mass (grams
or curies) per unit volume per unit time.
Profile = 1

 TIME (yrs) and Source Strength:  0 1E-5

 TIME (yrs) and Source Strength:  10 1E-5
```